

515

=>  
=> fil lreg

FILE 'LREGISTRY' ENTERED AT 10:55:18 ON 03 JUN 2004  
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LREGISTRY IS A STATIC LEARNING FILE

=> fil beilstein

FILE 'BEILSTEIN' ENTERED AT 10:55:23 ON 03 JUN 2004  
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FILE RELOADED ON OCTOBER 20, 2002  
FILE LAST UPDATED ON MARCH 30, 2004

FILE COVERS 1771 TO 2003.  
\*\*\* FILE CONTAINS 8,932,479 SUBSTANCES \*\*\*

>>> PLEASE NOTE: Reaction data and substance data are stored in  
separate documents and can not be searched together in one  
query.  
Reaction data for BEILSTEIN compounds may be displayed  
immediately with the display codes PRE (preparations) and REA  
(reactions). A substance answer set retrieved after the search  
for a chemical name, a molecular formula or a structure search  
for example can be restricted to compounds with available  
reaction information by concatenation with PRE/FA, REA/FA or  
more general with RX/FA. The BEILSTEIN Registry Number (BRN)  
is the link between a BEILSTEIN compound and belonging reactions.  
For more detailed reaction searches BRNs can be selected from  
substance answer sets and searched in the next step as reaction  
partner BRNs - Reactant (RX.RBRN) or Product BRN (RX.PBRN).  
After a search for reaction details substance documents  
associated with reactants or products may be retrieved by  
searching RX.PBRNs or RX.RBRNs as BRNs. <<<

>>> FOR SEARCHING PREPARATIONS SEE HELP PRE <<<

\*\*\*\*\*  
\* PLEASE NOTE THAT THERE ARE NO FORMATS FREE OF COST. \*  
\* SET NOTICE FEATURE: THE COST ESTIMATES CALCULATED FOR SET NOTICE \*  
\* ARE BASED ON THE HIGHEST PRICE CATEGORY. THEREFORE; THESE \*  
\* ESTIMATES MAY NOT REFLECT THE ACTUAL COSTS. \*  
\* FOR PRICE INFORMATION SEE HELP COST \*  
\*\*\*\*\*

=> d que l172  
L170 STR



REP G1=(1-2) CH2  
 NODE ATTRIBUTES:  
 CONNECT IS E3 RC AT 1  
 CONNECT IS E3 RC AT 3  
 CONNECT IS E1 RC AT 6  
 CONNECT IS E1 RC AT 7  
 DEFAULT MLEVEL IS ATOM  
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
 RING(S) ARE ISOLATED OR EMBEDDED  
 NUMBER OF NODES IS 9

STEREO ATTRIBUTES: NONE  
 L172 0 SEA FILE=BEILSTEIN SSS FUL L170

=> d que 1175

L171 STR



REP G1=(1-2) CH2  
 NODE ATTRIBUTES:  
 CONNECT IS E2 RC AT 1  
 CONNECT IS E3 RC AT 3  
 CONNECT IS E1 RC AT 6  
 CONNECT IS E1 RC AT 7  
 DEFAULT MLEVEL IS ATOM  
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
 RING(S) ARE ISOLATED OR EMBEDDED  
 NUMBER OF NODES IS 9

STEREO ATTRIBUTES: NONE  
 L173 4 SEA FILE=BEILSTEIN SSS FUL L171  
 L174 1 SEA FILE=BEILSTEIN ABB=ON PLU=ON L173 NOT RN/FA  
 L175 1 SEA FILE=BEILSTEIN ABB=ON PLU=ON L174 AND PY<1999

=> d 1175 ide

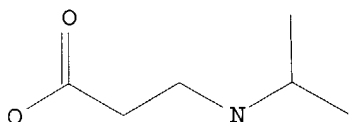
L175 ANSWER 1 OF 1 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Beilstein Records (BRN):	7957992
Chemical Name (CN):	3-isopropylamino-propionic acid; compound with trifluoro-acetic acid
Autonom Name (AUN):	3-isopropylamino-propionic acid; compound with trifluoro-acetic acid
Fragm. Molec. Formula (FMF):	C6 H13 N O2 , C2 H F3 O2
Molecular Formula (MF):	C6 H13 N O2 . C2 H F3 O2
Molecular Weight (MW):	131.17, 114.02
Fragment BRN (FBRN):	3043934, 742035
Lawson Number (LN):	3388, 2836, 1157

Compound Type (CTYPE): acyclic  
 Constitution ID (CONSID): 6821411  
 Tautomer ID (TAUTID): 7567547  
 Beilstein Citation (BSO): 6-04  
 Entry Date (DED): 1998/11/09  
 Update Date (DUPD): 1998/11/09

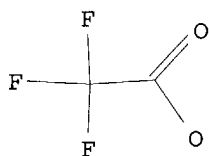
CM 1

FBRN 3043934  
 FMF C6 H13 N O2



CM 2

FBRN 742035  
 FMF C2 H F3 O2



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
FMF	Fragment Molecular Formula	2
MF	Molecular Formula	1
FW	Formular Weight	2
FBRN	Fragment BRN	2
LN	Lawson Number	3
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
ED	Entry Date	1
UPD	Update Date	1
NMR	Nuclear Magnetic Resonance	2

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
------	------	------------

```
=====
RX          Reaction Documents                      1
RXPRO       Substance is Reaction Product          1
```

=> d l175 rx

L175 ANSWER 1 OF 1 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Reaction:

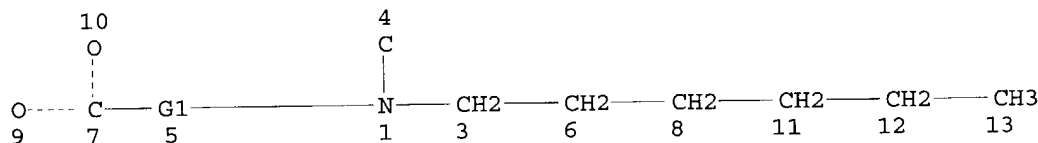
RX  
Reaction ID (.ID): 4887359  
Reactant BRN (.RBRN): 635744, 605259  
Reactant (.RCT): acryloyl chloride, isopropylamine  
Product BRN (.PBRN): 7957992  
Product (.PRO): 3-isopropylamino-propionic acid; compound  
with trifluoro-acetic acid  
No. of React. Details (.NVAR): 1

Reaction Details:

RX  
Reaction RID (.RID): 4887359.1  
Reaction Classification (.CL): Preparation  
Note(s) (.COM): Yield given. Multistep reaction  
Reference(s):  
1. Hamper, Bruce C.; Kolodziej, Stephen A.; Scates, Angela M.; Smith,  
Ronald G.; Cortez, Enriqueta, J.Org.Chem., CODEN: JOCEAH, 63(3),  
<1998>, 708-718; BABS-6090109

=> d que l185

L182 STR



REP G1=(1-2) CH2

NODE ATTRIBUTES:

CONNECT IS E3 RC AT 1

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 12

STEREO ATTRIBUTES: NONE

L183 5 SEA FILE=BEILSTEIN SSS FUL L182

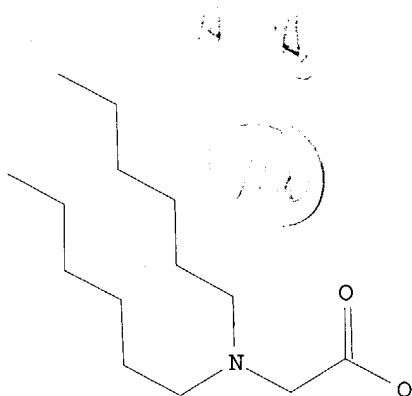
L184 2 SEA FILE=BEILSTEIN ABB=ON PLU=ON L183 NOT RN/FA

L185 2 SEA FILE=BEILSTEIN ABB=ON PLU=ON L184 AND PY<1999

=> d l185 ide 1

L185 ANSWER 1 OF 2 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Beilstein Records (BRN): 7917164  
 Chemical Name (CN): dihexylamino-acetic acid  
 Autonom Name (AUN): dihexylamino-acetic acid  
 Molec. Formula (MF): C14 H29 N O2  
 Molecular Weight (MW): 243.39  
 Lawson Number (LN): 3379, 2862  
 Compound Type (CTYPE): acyclic  
 Constitution ID (CONSID): 6761800  
 Tautomer ID (TAUTID): 7498208  
 Beilstein Citation (BSO): 6-04  
 Entry Date (DED): 1998/11/09  
 Update Date (DUPD): 1998/11/09



## Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	2
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
ED	Entry Date	1
UPD	Update Date	1
MP	Melting Point	1
NMR	Nuclear Magnetic Resonance	1

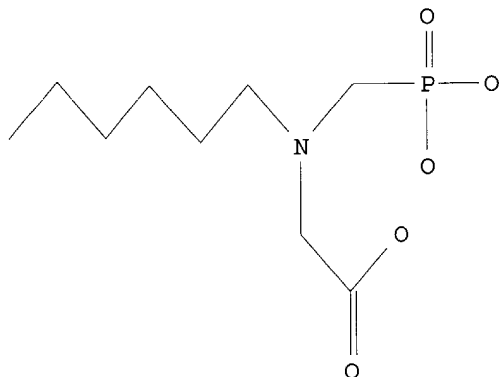
This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	2
RXREA	Substance is Reaction Reactant	1
RXPRO	Substance is Reaction Product	1

=> d 1185 ide 2

L185 ANSWER 2 OF 2 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Beilstein Records (BRN): 2271280  
 Chemical Name (CN): Hexyl-N-phosphonomethylglycinat  
 Autonom Name (AUN): (hexyl-phosphonomethyl-amino)-acetic acid  
 Molec. Formula (MF): C9 H20 N O5 P  
 Molecular Weight (MW): 253.23  
 Lawson Number (LN): 3379, 2862, 689  
 Compound Type (CTYPE): acyclic  
 Constitution ID (CONSID): 2090128  
 Tautomer ID (TAUTID): 2195791  
 Beilstein Citation (BSO): 5-04  
 Entry Date (DED): 1989/06/29  
 Update Date (DUPD): 1992/06/02



## Field Availability:

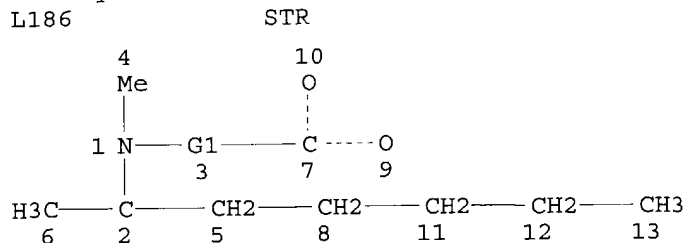
Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	3
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
ED	Entry Date	1
UPD	Update Date	1
MP	Melting Point	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
=====		

RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

=&gt; d que l188



REP G1=(1-2) CH2

NODE ATTRIBUTES:

CONNECT IS E3 RC AT 1

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

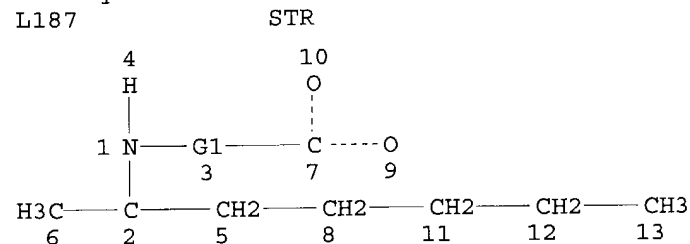
RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 13

STEREO ATTRIBUTES: NONE

L188 0 SEA FILE=BEILSTEIN SSS FUL L186

=&gt; d que l189



REP G1=(1-2) CH2

NODE ATTRIBUTES:

CONNECT IS E2 RC AT 1

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 13

STEREO ATTRIBUTES: NONE

L189 0 SEA FILE=BEILSTEIN SSS FUL L187

=&gt;

4/15

=> fil zcaplus

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FILE COVERS 1907 - 3 Jun 2004 VOL 140 ISS 23  
FILE LAST UPDATED: 2 Jun 2004 (20040602/ED)

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=> fil hcaplus

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=> fil biosis

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FILE COVERS 1969 TO DATE.  
CAS REGISTRY NUMBERS AND CHEMICAL NAMES (CNs) PRESENT  
FROM JANUARY 1969 TO DATE.

RECORDS LAST ADDED: 2 June 2004 (20040602/ED)



FILE RELOADED: 19 October 2003.

=> fil hcaplus

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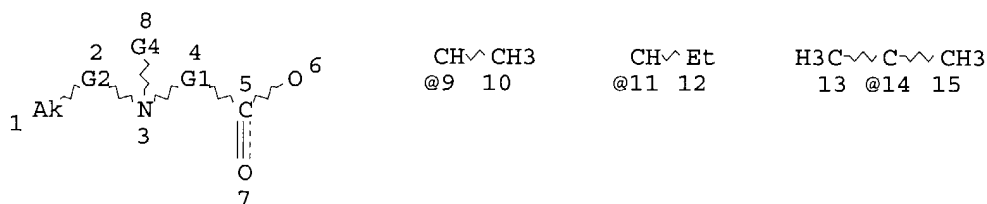
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FILE COVERS 1907 - 3 Jun 2004 VOL 140 ISS 23  
 FILE LAST UPDATED: 2 Jun 2004 (20040602/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d que 1153

L98 ( 1)SEA FILE=HCAPLUS ABB=ON PLU=ON (DURDEN, D? AND DAVIS, B? AND  
 DYCK, L? AND LIU, Y? AND BOULTON, A? AND PATERSON, I?)/AU  
 L99 SEL PLU=ON L98 1 RN : 103 TERMS  
 L100( 103)SEA FILE=REGISTRY ABB=ON PLU=ON L99  
 L101 SCR 1518  
 L102 SCR 2050 2052 2043  
 L103 SCR 1526  
 L104 SCR 1235  
 L105 STR



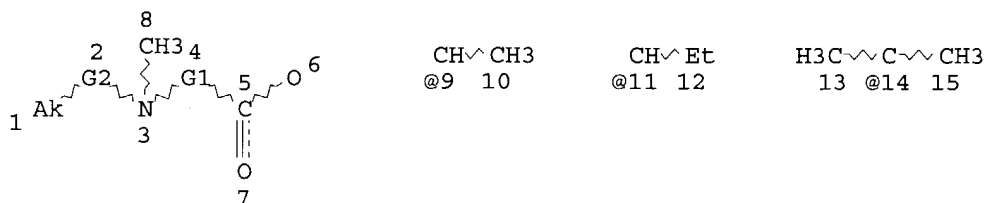
H<sub>3</sub>C~C~Et  
 16 @17 18

REP G1=(1-3) CH<sub>2</sub>  
 VAR G2=CH<sub>2</sub>/9/11/14/17  
 VAR G4=H/CH<sub>3</sub>  
 NODE ATTRIBUTES:  
 CONNECT IS E1 RC AT 1  
 CONNECT IS E1 RC AT 6  
 DEFAULT MLEVEL IS ATOM  
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
RING(S) ARE ISOLATED OR EMBEDDED  
NUMBER OF NODES IS 18

STEREO ATTRIBUTES: NONE

L106 SCR 963  
L107( 3584468)SEA FILE=REGISTRY ABB=ON PLU=ON N=1 NOT ((P/ELS OR SI/ELS)  
OR (TIS OR MNS OR AYS OR PMS)/CI OR SEQUENCE/FS)  
L108( 526)SEA FILE=REGISTRY SUB=L107 SSS FUL ((L101 AND L103 AND L104  
AND L106) NOT L102) AND L105  
L109( 37)SEA FILE=REGISTRY ABB=ON PLU=ON L100 NOT (?NITRILE? OR  
?PHOSPHONIC? OR ?AMINE? OR ?PROPENOIC? OR ?BROMO?)/CNS  
L110( 2)SEA FILE=REGISTRY ABB=ON PLU=ON L108 AND (C6 H13 N O2)/MF  
AND (?GLYCINE? AND ?METHYLETHYL? AND ?METHYL?)/CNS  
L111( 39)SEA FILE=REGISTRY ABB=ON PLU=ON L110 OR L109  
L112( 16)SEA FILE=REGISTRY ABB=ON PLU=ON (16217-35-9/CRN OR 244189-98-  
8/CRN OR 244189-99-9/CRN OR 244190-00-9/CRN OR 244190-01-0/CRN  
OR 244190-02-1/CRN OR 244190-03-2/CRN OR 244190-04-3/CRN OR  
27453-30-1/CRN OR 31044-47-0/CRN OR 3183-21-9/CRN OR 3183-22-0/  
CRN OR 41331-10-6/CRN OR 42313-51-9/CRN)  
L113( 41)SEA FILE=REGISTRY ABB=ON PLU=ON L111 OR L112  
L114( 18)SEA FILE=HCAPLUS ABB=ON PLU=ON L113 (L) (BIOL OR USES)/RL  
L115( 14)SEA FILE=HCAPLUS ABB=ON PLU=ON L114 AND (PY<1999 OR AY<1999  
OR PRY<1999)  
L116( 3)SEA FILE=HCAPLUS ABB=ON PLU=ON L115 NOT (PESTICIDE? OR  
PHOTOGRAPHIC? OR FOSSIL? OR INK? OR ALLOY? OR UNIT? OR  
NONCONDENSED?)/SC  
L117( 4)SEA FILE=HCAPLUS ABB=ON PLU=ON L114 NOT L115  
L118( 43)SEA FILE=HCAPLUS ABB=ON PLU=ON L113 (L) PREP/RL  
L119( 40)SEA FILE=HCAPLUS ABB=ON PLU=ON L118 AND (PY<1999 OR AY<1999  
OR PRY<1999)  
L120( 22)SEA FILE=HCAPLUS ABB=ON PLU=ON L119 AND PATENT/DT  
L121( 10)SEA FILE=HCAPLUS ABB=ON PLU=ON L120 AND US/PC.B  
L122 STR



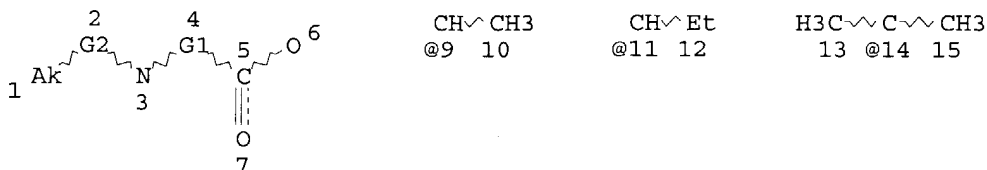
H3C~C~Et  
16 @17 18

REP G1=(1-3) CH2  
VAR G2=CH2/9/11/14/17  
NODE ATTRIBUTES:  
CONNECT IS E1 RC AT 1  
CONNECT IS E3 RC AT 3  
CONNECT IS E1 RC AT 6  
DEFAULT MLEVEL IS ATOM  
DEFAULT ECLEVEL IS LIMITED  
ECOUNT IS M1-X17 C AT 1

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED  
NUMBER OF NODES IS 18

STEREO ATTRIBUTES: NONE  
L123 STR



H3C~C~Et  
16 @17 18

REP G1=(1-3) CH2  
VAR G2=CH2/9/11/14/17  
NODE ATTRIBUTES:  
CONNECT IS E1 RC AT 1  
CONNECT IS E2 RC AT 3  
CONNECT IS E1 RC AT 6  
DEFAULT MLEVEL IS ATOM  
DEFAULT ECLEVEL IS LIMITED  
ECOUNT IS M1-X17 C AT 1

GRAPH ATTRIBUTES:  
RING(S) ARE ISOLATED OR EMBEDDED  
NUMBER OF NODES IS 17

STEREO ATTRIBUTES: NONE  
L124( 295)SEA FILE=REGISTRY SUB=L108 SSS FUL (L122 OR L123)  
L125( 598)SEA FILE=HCAPLUS ABB=ON PLU=ON L124 (L) (BIOL OR USES)/RL  
L126( 480)SEA FILE=HCAPLUS ABB=ON PLU=ON L125 AND (PY<1999 OR AY<1999  
OR PRY<1999)  
L127( 389)SEA FILE=HCAPLUS ABB=ON PLU=ON L126 AND PATENT/DT  
L128( 67)SEA FILE=HCAPLUS ABB=ON PLU=ON L127 AND US/PC.B  
L129( 25)SEA FILE=HCAPLUS ABB=ON PLU=ON L128 NOT (UNIT? OR LEATHER?  
OR DETERGENT? OR PHOTOGRAPHIC? OR FOSSIL? OR INK? OR ALLOY? OR  
EXPLOSIVE? OR PESTICID? OR WOOD? OR PETROLEUM? OR INORGANIC?  
OR PLASTIC?)/SC  
L130( 25)SEA FILE=HCAPLUS ABB=ON PLU=ON L129 NOT ((L116 OR L117))  
L131( 24)SEA FILE=HCAPLUS ABB=ON PLU=ON L130 NOT (AGRO?)/SC  
L132( 12)SEA FILE=HCAPLUS ABB=ON PLU=ON L131 AND (COSMET?)/SC  
L133( 12)SEA FILE=HCAPLUS ABB=ON PLU=ON L131 NOT L132  
L134( 126)SEA FILE=HCAPLUS ABB=ON PLU=ON L124 (L) PREP/RL  
L135( 106)SEA FILE=HCAPLUS ABB=ON PLU=ON L134 AND (PY<1999 OR AY<1999  
OR PRY<1999)  
L136( 52)SEA FILE=HCAPLUS ABB=ON PLU=ON L135 AND PATENT/DT  
L137( 10)SEA FILE=HCAPLUS ABB=ON PLU=ON L136 AND US/PC.B  
L138( 5)SEA FILE=HCAPLUS ABB=ON PLU=ON L137 NOT L121  
L139( 10)SEA FILE=HCAPLUS ABB=ON PLU=ON L121 NOT L116  
L140( 12)SEA FILE=HCAPLUS ABB=ON PLU=ON L133 NOT L116  
L141( 4)SEA FILE=HCAPLUS ABB=ON PLU=ON L138 NOT (L116 OR L133)  
L142( 55)SEA FILE=HCAPLUS ABB=ON PLU=ON "DYCK L E"/AU OR ("DYCK  
LILIAN E"/AU OR "DYCK LILLIAN"/AU OR "DYCK LILLIAN E"/AU OR  
"DYCK LILLIAN EVA"/AU)  
L143( 184)SEA FILE=HCAPLUS ABB=ON PLU=ON DAVIS/AU OR ("DAVIS B"/AU OR

"DAVIS B A"/AU)  
 L144 ( 1591) SEA FILE=HCAPLUS ABB=ON PLU=ON "LIU Y"/AU OR "LIU Y D"/AU OR  
 "LIU YA DONG"/AU  
 L145 ( 80) SEA FILE=HCAPLUS ABB=ON PLU=ON ("DURDEN D"/AU OR "DURDEN D  
 A"/AU) OR ("DURDEN DAVE A"/AU OR "DURDEN DAVID"/AU OR "DURDEN  
 DAVID A"/AU)  
 L146 ( 341) SEA FILE=HCAPLUS ABB=ON PLU=ON ("BOULTON A"/AU OR "BOULTON A  
 A"/AU) OR ("BOULTON ALAN"/AU OR "BOULTON ALAN A"/AU)  
 L147 ( 4) SEA FILE=HCAPLUS ABB=ON PLU=ON PETERSON/AU OR ("PETERSON  
 I"/AU OR "PETERSON I ALICK"/AU)  
 L148 ( 527) SEA FILE=HCAPLUS ABB=ON PLU=ON KENNEDY/AU OR ("KENNEDY B"/AU  
 OR "KENNEDY B A"/AU OR "KENNEDY B C"/AU OR "KENNEDY B F"/AU OR  
 "KENNEDY B G"/AU OR "KENNEDY B H"/AU OR "KENNEDY B J"/AU OR  
 "KENNEDY B L"/AU OR "KENNEDY B M"/AU OR "KENNEDY B MACK"/AU OR  
 "KENNEDY B P"/AU OR "KENNEDY B P C"/AU OR "KENNEDY B R"/AU OR  
 "KENNEDY B S"/AU OR "KENNEDY B W"/AU) OR ("KENNEDY BRENDA  
 J"/AU OR "KENNEDY BRENDA SCHAFER"/AU OR "KENNEDY BRENDA V"/AU)  
 L149 ( 238) SEA FILE=HCAPLUS ABB=ON PLU=ON ("ROGERS K"/AU OR "ROGERS K  
 A"/AU OR "ROGERS K B"/AU OR "ROGERS K C"/AU OR "ROGERS K D"/AU  
 OR "ROGERS K E"/AU OR "ROGERS K F"/AU OR "ROGERS K H"/AU OR  
 "ROGERS K J"/AU OR "ROGERS K L"/AU OR "ROGERS K M"/AU OR  
 "ROGERS K N"/AU OR "ROGERS K R"/AU OR "ROGERS K S"/AU OR  
 "ROGERS K T"/AU OR "ROGERS K V"/AU OR "ROGERS K W"/AU) OR  
 ("ROGERS KEVIN"/AU OR "ROGERS KEVIN B"/AU OR "ROGERS KEVIN  
 BONZI"/AU OR "ROGERS KEVIN J"/AU OR "ROGERS KEVIN M"/AU OR  
 "ROGERS KEVIN P"/AU OR "ROGERS KEVIN PHILIP"/AU OR "ROGERS  
 KEVIN PHILLIP"/AU OR "ROGERS KEVIN R"/AU)  
 L150 ( 2900) SEA FILE=HCAPLUS ABB=ON PLU=ON (L142 OR L143 OR L144 OR L145  
 OR L146 OR L147 OR L148 OR L149)  
 L151 ( 1552) SEA FILE=HCAPLUS ABB=ON PLU=ON L150 AND (PY<1999 OR PRY<1999  
 OR AY<1999)  
 L152 ( 4) SEA FILE=HCAPLUS ABB=ON PLU=ON L151 AND (?SASKATCHEWAN?)/SO,P  
 A  
 L153 3 SEA FILE=HCAPLUS ABB=ON PLU=ON L152 NOT (L116 OR L139 OR  
 L140 OR L141)

=> s l153 not (l38 or l97)

L168 3 L153 NOT (L38 OR L97)

=> FIL STNGUIDE

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FILE CONTAINS CURRENT INFORMATION.

LAST RELOADED: May 28, 2004 (20040528/UP).

d que l167

L154 ( 79) SEA FILE=BIOSIS ABB=ON PLU=ON "DYCK L"/AU OR "DYCK L E"/AU  
 OR ("DYCK LILLIAN"/AU OR "DYCK LILLIAN E"/AU)  
 L155 ( 553) SEA FILE=BIOSIS ABB=ON PLU=ON DAVIS/AU OR ("DAVIS B"/AU OR  
 "DAVIS B A"/AU) OR ("DAVIS BRUCE"/AU OR "DAVIS BRUCE A"/AU)  
 L156 ( 3449) SEA FILE=BIOSIS ABB=ON PLU=ON LIU/AU OR ("LIU Y"/AU OR "LIU  
 Y A"/AU OR "LIU Y B"/AU OR "LIU Y C"/AU OR "LIU Y C L"/AU OR  
 "LIU Y D"/AU OR "LIU Y DIANA"/AU OR "LIU Y E"/AU OR "LIU Y  
 F"/AU OR "LIU Y FANG"/AU OR "LIU Y G"/AU OR "LIU Y H"/AU OR  
 "LIU Y I"/AU OR "LIU Y J"/AU OR "LIU Y K"/AU OR "LIU Y L"/AU  
 OR "LIU Y LUCY"/AU OR "LIU Y M"/AU OR "LIU Y N"/AU OR "LIU Y N

C"/AU OR "LIU Y O"/AU OR "LIU Y P"/AU OR "LIU Y Q"/AU OR "LIU Y Q E"/AU OR "LIU Y R"/AU OR "LIU Y S"/AU OR "LIU Y S V"/AU OR "LIU Y SHIUAN"/AU OR "LIU Y SR"/AU OR "LIU Y T"/AU OR "LIU Y W"/AU OR "LIU Y X"/AU OR "LIU Y Y"/AU OR "LIU Y YI"/AU OR "LIU Y YONG"/AU OR "LIU Y YU"/AU OR "LIU Y Z"/AU OR "LIU Y ZHEN"/AU OR "LIU YA"/AU) OR "LIU YA DONG"/AU

L157( 81)SEA FILE=BIOSIS ABB=ON PLU=ON ("DURDEN D"/AU OR "DURDEN D A"/AU) OR ("DURDEN DAVID"/AU OR "DURDEN DAVID A"/AU)

L158( 390)SEA FILE=BIOSIS ABB=ON PLU=ON ("BOULTON A"/AU OR "BOULTON A A"/AU) OR ("BOULTON ALAN"/AU OR "BOULTON ALAN A"/AU)

L159( 13)SEA FILE=BIOSIS ABB=ON PLU=ON ("PETERSON I"/AU OR "PETERSON I A"/AU) OR "PETERSON IAN"/AU

L160( 839)SEA FILE=BIOSIS ABB=ON PLU=ON KENNEDY/AU OR ("KENNEDY B"/AU OR "KENNEDY B B"/AU OR "KENNEDY B C"/AU OR "KENNEDY B D"/AU OR "KENNEDY B E"/AU OR "KENNEDY B F"/AU OR "KENNEDY B G"/AU OR "KENNEDY B H"/AU OR "KENNEDY B J"/AU OR "KENNEDY B K"/AU OR "KENNEDY B L"/AU OR "KENNEDY B M"/AU OR "KENNEDY B N"/AU OR "KENNEDY B P"/AU OR "KENNEDY B P C"/AU OR "KENNEDY B R"/AU OR "KENNEDY B R C"/AU OR "KENNEDY B S"/AU OR "KENNEDY B V"/AU OR "KENNEDY B W"/AU) OR "KENNEDY BRENDA"/AU

L161( 609)SEA FILE=BIOSIS ABB=ON PLU=ON ("ROGERS K"/AU OR "ROGERS K A"/AU OR "ROGERS K B"/AU OR "ROGERS K C"/AU OR "ROGERS K D"/AU OR "ROGERS K E"/AU OR "ROGERS K F"/AU OR "ROGERS K G"/AU OR "ROGERS K H"/AU OR "ROGERS K J"/AU OR "ROGERS K K"/AU OR "ROGERS K L"/AU OR "ROGERS K M"/AU OR "ROGERS K P"/AU OR "ROGERS K R"/AU OR "ROGERS K S"/AU OR "ROGERS K T"/AU OR "ROGERS K V"/AU OR "ROGERS K W"/AU) OR ("ROGERS KEVIN"/AU OR "ROGERS KEVIN B"/AU OR "ROGERS KEVIN H"/AU OR "ROGERS KEVIN L"/AU OR "ROGERS KEVIN M"/AU OR "ROGERS KEVIN R"/AU)

L162( 5836)SEA FILE=BIOSIS ABB=ON PLU=ON (L154 OR L155 OR L156 OR L157 OR L158 OR L159 OR L160 OR L161)

L163( 4685)SEA FILE=BIOSIS ABB=ON PLU=ON L162 AND (PY<1999 OR MY<1999)

L164( 163)SEA FILE=BIOSIS ABB=ON PLU=ON L163 AND ?SASKATCHEWAN?/CS,SO

L165( 8)SEA FILE=BIOSIS ABB=ON PLU=ON L164 AND (?APOPTO? OR ANTIAPOPT O?)

L166( 3)SEA FILE=BIOSIS ABB=ON PLU=ON L164 AND (?CELL? (5A) (?RESCU? OR ?DEATH?))

L167 11 SEA FILE=BIOSIS ABB=ON PLU=ON L165 OR L166

=> dup rem l168 l167

FILE 'HCAPLUS' ENTERED AT 08:52:53 ON 03 JUN 2004  
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 PROCESSING COMPLETED FOR L168  
 PROCESSING COMPLETED FOR L167  
 L169 13 DUP REM L168 L167 (1 DUPLICATE REMOVED)  
 ANSWERS '1-3' FROM FILE HCAPLUS  
 ANSWERS '4-13' FROM FILE BIOSIS

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=&gt; d l169 ibib abs 1-3

L169 ANSWER 1 OF 13 HCAPLUS COPYRIGHT 2004 ACS on STN DUPLICATE 1  
ACCESSION NUMBER: 1998:774327 HCAPLUS  
DOCUMENT NUMBER: 129:343272  
TITLE: Preparation of aliphatic propargylamines as neuroprotective agents  
INVENTOR(S): Durden, David; Paterson, Alick; Davis, Bruce; Dyck, Lillian; Yu, Peter; Li, Xinmin; Boulton, Alan  
PATENT ASSIGNEE(S): University of Saskatchewan, Can.  
SOURCE: U.S., 12 pp.  
CODEN: USXXAM  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5840979	A	19981124	US 1997-891904	19970714 <--
US 6251950	B1	20010626	US 1998-110548	19980706 <--
WO 9903817	A2	19990128	WO 1998-CA683	19980714 <--
WO 9903817	A3	19990527		
W:	AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
AU 9883289	A1	19990210	AU 1998-83289	19980714 <--
EP 996612	A2	20000503	EP 1998-933408	19980714 <--
EP 996612	B1	20030409		
R:	DE, FR, GB, IT			
JP 2001510179	T2	20010731	JP 2000-503049	19980714 <--
PRIORITY APPLN. INFO.:			US 1997-891904	A3 19970714 <--
			WO 1998-CA683	W 19980714 <--

OTHER SOURCE(S): MARPAT 129:343272  
AB Aliphatic propargylamines HC.tplbond.CCH2NHCH(R1)R2 [R1 = H, CH3; R2 = CH3(CH2)n; n = 0-16; such that if R1 = H then n >4, if R1 = CH3 then n ≠ 0, and if R1 = CH3 and n = 1-4 then the title compound is in the form of a pure enantiomer in the (R)-configuration] and their salts, useful as neuroprotective and anti-ischemic agents in the treatment and prevention of cell death by apoptosis, are prepared. Thus, (R)-2-heptylamine (prepared by the resolution of 2-heptylamine) was condensed with propargyl bromide and salified with HCl, producing (R)-N-2-heptylpropargylamine hydrochloride which demonstrated a 230 ± 36% (at 0.1 mg/kg, p.o.) survival in a rat model of apoptosis of hippocampal pyramidal neurons by hypoxia/ischemia, vs. 100 ± 22% survival for water.  
REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L169 ANSWER 2 OF 13 HCAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 1999:468566 HCAPLUS  
DOCUMENT NUMBER: 131:111423  
TITLE: Composition containing a propargylamine for enhancing cancer therapy  
INVENTOR(S): Paterson, I. Alick; Boulton, Alan A.

PATENT ASSIGNEE(S): University of **Saskatchewan** Technologies  
Inc., Can.; The Canada Trust Company; Warrington, R.  
C.  
SOURCE: PCT Int. Appl., 36 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

*WIP*

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9936076	A1	19990722	WO 1999-CA5	19990113 <--
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2318693	AA	19990722	CA 1999-2318693	19990113 <--
AU 9919563	A1	19990802	AU 1999-19563	19990113 <--
EP 1049478	A1	20001108	EP 1999-900405	19990113 <--
EP 1049478	B1	20020904		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
AT 223209	E	20020915	AT 1999-900405	19990113 <--
HK 1032204	A1	20030509	HK 2001-102511	20010410 <--
PRIORITY APPLN. INFO.:			US 1998-71023P	P 19980113 <--
			WO 1999-CA5	W 19990113
OTHER SOURCE(S):		MARPAT 131:111423		
AB Antineoplastic drug modulators are described. The specific modulators referred to are propargylamines which can enhance the cytotoxic effects of antineoplastic drugs on cancer cells while protecting normal cells from damage. The propargylamine modulators can be used to increase the selectivity and effectiveness of conventional antineoplastic drugs, to reduce the unwanted side-effects of cancer chemotherapy, to improve effectiveness of cancer chemotherapy, to improve treatment of cancers for which treatment is otherwise ineffective, to improve therapy of cancers otherwise unresponsive or poorly responsive due to drug-resistance and/or toxicity limited treatment regimens and to render effective chemotherapy for previously untreatable cancers.				
REFERENCE COUNT:		2	THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT	
L169 ANSWER 3 OF 13 HCAPLUS COPYRIGHT 2004 ACS on STN				
ACCESSION NUMBER:		1993:59281 HCAPLUS		
DOCUMENT NUMBER:		118:59281		
TITLE:		Preparation of aliphatic propargylamines as selective MAO-B inhibitors and neuroprotective agents		
INVENTOR(S):		Yu, Peter H.; Davis, Bruce A.; <b>Boulton, Alan A.</b>		
PATENT ASSIGNEE(S):		University of <b>Saskatchewan</b> , Can.		
SOURCE:		PCT Int. Appl., 81 pp. CODEN: PIXXD2		
DOCUMENT TYPE:		Patent		
LANGUAGE:		English		
FAMILY ACC. NUM. COUNT:		1		

## PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9215551	A1	19920917	WO 1992-CA90	19920228 <--
W: AT, AU, BB, BG, BR, CA, CH, CS, DE, DK, ES, FI, GB, HU, JP, KP, KR, LK, LU, MG, MN, MW, NL, NO, PL, RO, RU, SD, SE, US				
RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FR, GA, GB, GN, GR, IT, LU, MC, ML, MR, NL, SE, SN, TD, TG				
US 5169868	A	19921208	US 1991-663018	19910301 <--
AU 9213236	A1	19921006	AU 1992-13236	19920228 <--
AU 658611	B2	19950427		
EP 573498	A1	19931215	EP 1992-905512	19920228 <--
EP 573498	B1	19981118		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, MC, NL, SE				
JP 06505241	T2	19940616	JP 1992-504826	19920228 <--
JP 3129733	B2	20010131		
AT 173459	E	19981215	AT 1992-905512	19920228 <--
US 5508311	A	19960416	US 1993-108653	19931223 <--
HK 1014533	A1	20000505	HK 1998-115865	19981228 <--
PRIORITY APPLN. INFO.:				
			US 1991-663018	A2 19910301 <--
			US 1991-633018	A 19910301 <--
			WO 1992-CA90	A 19920228 <--

OTHER SOURCE(S): MARPAT 118:59281

AB R2CHR1NMECH2C.tplbond.CH (I; R1 = H, alkyl; R2 = (substituted) C3-11 alkyl, -alkenyl, -alkynyl, -alkynyl, -alkoxy, -alkylthio, -alkylsulfinyl; with provisos), are prepared Me(CH2)2CH2Br, CH.tplbond.CCH2NHMe and anhydrous Na2CO3 were heated for 72 h in EtOH to give I (R1 = H, R2 = Pr).HCl (II). II inhibited MAO-B activity in mouse brain with ID50 = 2 mg/kg i.p.

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YOU HAVE REQUESTED DATA FROM 10 ANSWERS - CONTINUE? Y/(N):y


L169 ANSWER 4 OF 13 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN  
ACCESSION NUMBER: 1998:124820 BIOSIS  
DOCUMENT NUMBER: PREV199800124820  
TITLE: R-Deprenyl and R-2-Heptyl-N-methylpropargylamine prevent **apoptosis** in cerebellar granule neurons induced by cytosine arabinoside but not low extracellular potassium.  
AUTHOR(S): Paterson, I. A. [Reprint author]; Zhang, D.; Warrington, R. C.; Boulton, A. A.  
CORPORATE SOURCE: Neuropsychiatry Res. Unit, Dep. Psychiatry, A114 Med. Res. Build., Univ. Saskatchewan, 103 Wiggins Road, Saskatoon, Saskatchewan S7N 5E4, Canada  
SOURCE: Journal of Neurochemistry, (Feb., 1998) Vol. 70, No. 2, pp. 515-523. print.  
CODEN: JONRA9. ISSN: 0022-3042.  
DOCUMENT TYPE: Article  
LANGUAGE: English  
ENTRY DATE: Entered STN: 5 Mar 1998  
Last Updated on STN: 5 Mar 1998

AB R-Deprenyl and R-2-heptyl-N-methylpropargylamine (R-2-HMP) are compounds that have been shown to reduce neuronal death in various in vitro and in vivo models involving **apoptosis** but do not always prevent **apoptosis**. In the present study we have examined the effects of these compounds and their S enantiomers on cytosine arabinoside (ara C)-induced **apoptosis** and low K+-induced **apoptosis** in cerebellar granule cells in primary culture. It was found that R-deprenyl and R-2-HMP could prevent ara C-induced **apoptosis** with an EC50



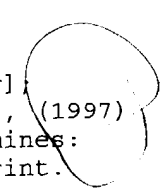
around  $10^{-9}$  M but could not prevent low  $K^{+}$ -induced **apoptosis**. S-Deprenyl and S-2-HMP did not prevent **apoptosis** under any conditions but were found to antagonize the **antiapoptotic** actions of R-deprenyl and R-2-HMP. Using the fluorescent mitochondrial dye chloromethyltetramethylrhodamine methyl ester it was found that there was a loss of mitochondrial function in cerebellar granule cells exposed to ara C but not low  $K^{+}$  medium. R-Deprenyl and R-2-HMP prevented the ara C-induced loss of mitochondrial function. It is concluded that R-deprenyl and R-2-HMP prevent **apoptosis** of cerebellar granule cells by a mechanism that is independent of monoamine oxidase inhibition and that they act on the same site to prevent specifically **apoptosis** involving a loss of mitochondrial membrane potential, possibly p53-dependent **apoptosis**.

L169 ANSWER 5 OF 13 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN  
ACCESSION NUMBER: 1999:283898 BIOSIS  
DOCUMENT NUMBER: PREV199900283898  
TITLE: L-deprenyl induces aromatic L-amino acid decarboxylase (AADC) mRNA in the rat substantia nigra and ventral tegmentum: An in situ hybridization study.  
AUTHOR(S): Li, Xin-Min [Reprint author]; Juorio, Augusto V.; Qi, Jin; Boulton, Alan A.  
CORPORATE SOURCE: Neuropsychiatry Research Unit, Department of Psychiatry, University of Saskatchewan, Saskatoon, SK, S7N 5E4, Canada  
SOURCE: Molecular and Chemical Neuropathology, (Aug.-Dec., 1998) Vol. 35, No. 1-3, pp. 149-155. print. ISSN: 1044-7393.  
DOCUMENT TYPE: Article  
LANGUAGE: English  
ENTRY DATE: Entered STN: 28 Jul 1999  
Last Updated on STN: 28 Jul 1999



AB L-Deprenyl is a complex drug, and number of mechanisms have been proposed to explain its effects. These include blockade of dopamine metabolism, amplification of dopamine responses, induction of superoxide dismutase or delaying **apoptosis**. Using in situ hybridization techniques, we have shown that L-deprenyl (5-10 mg/kg intraperitoneally, killed after 24 h) increases aromatic L-amino acid decarboxylase (AADC) mRNA levels in rat substantia nigra/ventral tegmental area. In human brain tissue, AADC is present at low levels, suggesting a possible rate-limiting role in monoamine synthesis. This is particularly important in parkinsonian patients, since the therapeutic efficacy of L-DOPA is attributed to its enzymatic decarboxylation to dopamine. The present findings support that one of the effects of L-deprenyl may be to facilitate the decarboxylation of L-DOPA by increasing the availability, of AADC.

L169 ANSWER 6 OF 13 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN  
ACCESSION NUMBER: 1998:26851 BIOSIS  
DOCUMENT NUMBER: PREV199800026851  
TITLE: Aliphatic N-methylpropargylamines: Monoamine oxidase-B inhibitors and **antiapoptotic** drugs.  
AUTHOR(S): Boulton, Alan A.; Yu, Peter H.; Davis, Bruce A.; Paterson, I. Alick; Li, Xi-Min; Juorio, Augusto V.; Durden, David A.; Dyck, Lillian E.  
CORPORATE SOURCE: Neuropsychiatry Res. Unit, Univ. Saskatchewan, Saskatoon, SK S7N 5E4, Canada  
SOURCE: Goldstein, D. S. [Editor]; Eisenhofer, G. [Editor]; McCarty, R. [Editor]. Adv. Pharmacol. (San Diego), (1997) pp. 308-311. Advances in Pharmacology; Catecholamines: Bridging basic science with clinical medicine. print.



Publisher: Academic Press, Inc., 1250 Sixth Ave., San Diego, California 92101, USA; Academic Press Ltd., 14 Belgrave Square, 24-28 Oval Road, London NW1 70X, England, UK. Series: Advances in Pharmacology.

Meeting Info.: Eighth International Catecholamine Symposium. Pacific Grove, California, USA. October 13-18, 1996.

CODEN: ADPHEL. ISSN: 1054-3589. ISBN: 0-12-032943-3.

## DOCUMENT TYPE:

Book  
Conference; (Meeting)  
Book; (Book Chapter)  
Conference; (Meeting Paper)

## LANGUAGE:

English

## ENTRY DATE:

Entered STN: 5 Jan 1998  
Last Updated on STN: 24 Feb 1998

L169 ANSWER 7 OF 13 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN

ACCESSION NUMBER: 1997:533932 BIOSIS

DOCUMENT NUMBER: PREV199799833135

TITLE: The anti-**apoptotic** effects of 2HMP is due to a desmethyl metabolite.

AUTHOR(S): Paterson, I. A.; **Dyck, L. E.; Durden, D. A.; Davis, B. A.; Liu, Y.; Boulton, A. A.**

CORPORATE SOURCE: Neuropsychiatry, Res. Unit, Dep. Psychiatry, Univ. **Saskatchewan**, Saskatoon, SK S7N 5E4, Canada

SOURCE: Society for Neuroscience Abstracts, (1997) Vol. 23, No. 1-2, pp. 2254.  
Meeting Info.: 27th Annual Meeting of the Society for Neuroscience. New Orleans, Louisiana, USA. October 25-30, 1997.

ISSN: 0190-5295.

## DOCUMENT TYPE:

Conference; (Meeting)  
Conference; Abstract; (Meeting Abstract)  
Conference; (Meeting Poster)

## LANGUAGE:

English

## ENTRY DATE:

Entered STN: 12 Dec 1997  
Last Updated on STN: 12 Dec 1997

L169 ANSWER 8 OF 13 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN

ACCESSION NUMBER: 1998:275926 BIOSIS

DOCUMENT NUMBER: PREV199800275926

TITLE: Aliphatic propargylamines: New **antiapoptotic** drugs.

AUTHOR(S): **Boulton, Alan A.** [Reprint author]; **Davis, Bruce A.; Durden, David A.; Dyck, Lillian E.**; Juorio, Augusto V.; Li, Xin-Min; Paterson, I. Alick; Yu, Peter H.

CORPORATE SOURCE: Neuropsychiatry Res. Unit, A114 Med. Res. Build., Univ. **Saskatchewan**, 103 Wiggins Road, Saskatoon, SK S7N 5E4, Canada

SOURCE: Drug Development Research, (Nov.-Dec., 1997) Vol. 42, No. 3-4, pp. 150-156. print.  
CODEN: DDREDK. ISSN: 0272-4391.

## DOCUMENT TYPE:

Article  
General Review; (Literature Review)

## LANGUAGE:

English

## ENTRY DATE:

Entered STN: 24 Jun 1998  
Last Updated on STN: 13 Aug 1998

AB Two series of drugs, the aliphatic-N-methyl propargylamines and the

aliphatic propargylamines, have been synthesised and shown to be specific, irreversible, and potent monoamine oxidase B inhibitors and neural rescue agents. In the latter case, an absolute stereochemical requirement for the R isomer exists. Both series of compounds have been shown, in numerous in vitro and in vivo experimental paradigms, to be effective neuronal rescue agents. Candidates from both series exhibit excellent bioavailability and pharmacokinetics and offer opportunities for treating neurodegenerative disorders and stroke and cognitive decline in companion animals.

L169 ANSWER 9 OF 13 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN  
ACCESSION NUMBER: 1997:382572 BIOSIS  
DOCUMENT NUMBER: PREV199799681775  
TITLE: R-deprenyl and R-2-heptylmethylpropargylamine prevent P53-dependent but not P53-independent **apoptosis**.  
AUTHOR(S): Paterson, I. A.; Warrington, R.; **Boulton, A. A.**  
CORPORATE SOURCE: Neuropsychiatry Res. Unit, Univ. **Saskatchewan**, 103 Wiggins Road, Saskatoon, SK S7N 5E4, Canada  
SOURCE: Journal of Neurochemistry, (1997) Vol. 69, No. SUPPL., pp. S137.  
Meeting Info.: Joint Sixteenth Biennial Meeting of the International Society for Neurochemistry and Twenty-eighth Annual Meeting of the American Society for Neurochemistry. Boston, Massachusetts, USA. July 20-26, 1997.  
CODEN: JONRA9. ISSN: 0022-3042.  
DOCUMENT TYPE: Conference; (Meeting)  
Conference; Abstract; (Meeting Abstract)  
LANGUAGE: English  
ENTRY DATE: Entered STN: 4 Sep 1997  
Last Updated on STN: 4 Sep 1997

L169 ANSWER 10 OF 13 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN  
ACCESSION NUMBER: 1996:527439 BIOSIS  
DOCUMENT NUMBER: PREV199699249795  
TITLE: MK-801 induces **apoptotic** neuronal death in the rat retrosplenial cortex: Prevention by cycloheximide and R(-)-2-hexyl-N-methylpropargylamine.  
AUTHOR(S): Zhang, Xia; **Boulton, Alan A.**; Zuo, Dong-Mei; Yu, Peter H. [Reprint author]  
CORPORATE SOURCE: Neuropsychiatry Res. Unit, Dep. psychiatry, Univ. **Saskatchewan**, Saskatoon, **Saskatchewan** S7N 5E4, Canada  
SOURCE: Journal of Neuroscience Research, (1996) Vol. 46, No. 1, pp. 82-89.  
CODEN: JNREDK. ISSN: 0360-4012.  
DOCUMENT TYPE: Article  
LANGUAGE: English  
ENTRY DATE: Entered STN: 22 Nov 1996  
Last Updated on STN: 23 Nov 1996

AB MK-801 is a non-competitive N-methyl-D-aspartate (NMDA) receptor antagonist which can prevent excitatory neuronal death. At higher concentrations, however, it can also induce neuronal death in the limbic system. This MK-801-induced selective neurotoxicity has been proposed as an animal model for dementia and psychosis. We have investigated the effects of the protein synthesis inhibitor cycloheximide and the neurorescue agent 2-hexyl-N-methylpropargylamine (R(-)-2HxMP) on MK-801-induced neuronal death in the retrosplenial cortex in the rat. Cycloheximide (2 mg/kg, subcutaneously (sc)) administered either 1 hr before, or after, injection of MK801 (5 mg/kg, sc) prevented almost completely neuronal shrinkage and nuclear condensation of the granular

retrosplenial cortex as assessed by hematoxylin-eosin staining. The results suggest that the MK801-induced neuronal death was **apoptotic**. This neurorescue effect by cycloheximide was time dependent: after 4 hr the effect was reduced to about 50% and by 8 hr had disappeared. R(-)-2HxMP (0.25 mg/kg, sc), which does not inhibit protein synthesis in vitro, was also found to be effective at preventing MK-801-induced neuronal death.

L169 ANSWER 11 OF 13 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN  
ACCESSION NUMBER: 1996:493093 BIOSIS  
DOCUMENT NUMBER: PREV199699215449  
TITLE: MK-801-induced expression of BCL-2, Fos and HSP72 proteins in the rat cerebral cortex.  
AUTHOR(S): Zhang, X.; Fan, X.; Yu, P. H.; **Boulton, A. A.**  
CORPORATE SOURCE: Neuropsychiatry Res. Unit, Dep. Psychiatry, Univ. **Saskatchewan**, Saskatoon, SK S7N 5E4, Canada  
SOURCE: Society for Neuroscience Abstracts, (1996) Vol. 22, No. 1-3, pp. 42.  
Meeting Info.: 26th Annual Meeting of the Society for Neuroscience. Washington, D.C., USA. November 16-21, 1996. ISSN: 0190-5295.  
DOCUMENT TYPE: Conference; (Meeting)  
Conference; Abstract; (Meeting Abstract)  
Conference; (Meeting Poster)  
LANGUAGE: English  
ENTRY DATE: Entered STN: 4 Nov 1996  
Last Updated on STN: 5 Nov 1996

L169 ANSWER 12 OF 13 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN  
ACCESSION NUMBER: 1995:147634 BIOSIS  
DOCUMENT NUMBER: PREV199598161934  
TITLE: Neuroprotective effects of N-methylpropargylamines against kainic acid induced neuronal damage in the rat brain.  
AUTHOR(S): Zhang, X.; Yu, P. H.; **Davis, B. A.**; Zuo, C. T.; **Boulton, A. A.**  
CORPORATE SOURCE: Neuropsychiatry Res. Unit, Univ. **Saskatchewan**, Saskatoon S7N 0W0, Canada  
SOURCE: Journal of Neurochemistry, (1995) Vol. 64, No. SUPPL. 1, pp. S96.  
Meeting Info.: Twenty-sixth Meeting of the American Society for Neurochemistry. Santa Monica, California, USA. March 5-9, 1995.  
CODEN: JONRA9. ISSN: 0022-3042.  
DOCUMENT TYPE: Conference; (Meeting)  
Conference; Abstract; (Meeting Abstract)  
LANGUAGE: English  
ENTRY DATE: Entered STN: 3 Apr 1995  
Last Updated on STN: 23 May 1995

L169 ANSWER 13 OF 13 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN  
ACCESSION NUMBER: 1994:535587 BIOSIS  
DOCUMENT NUMBER: PREV199497548587  
TITLE: Neuroprotective effects of some monoamine oxidase-B inhibitors against DSP-4-induced noradrenaline depletion in the mouse hippocampus.  
AUTHOR(S): Yu, P. H. [Reprint author]; **Davis, B. A.**; Fang, J.; **Boulton, A. A.**  
CORPORATE SOURCE: Neuropsychiatric Res. Unit, Dep. Psychiatry, Univ. **Saskatchewan**, Saskatoon, SK S7N 0W0, Canada  
SOURCE: Journal of Neurochemistry, (1994) Vol. 63, No. 5, pp.

1820-1828.

CODEN: JONRA9. ISSN: 0022-3042.

DOCUMENT TYPE:

Article

LANGUAGE:

English

ENTRY DATE:

Entered STN: 15 Dec 1994

Last Updated on STN: 16 Dec 1994

AB DSP-4 (N-(2-chloroethyl)-N-ethyl-2-bromobenzylamine), a selective noradrenaline (NA) uptake blocker, is capable of inducing long-lasting depletion of NA in some noradrenergic axon terminals and of subsequently causing **cell death** to NA neuronal **cell** bodies in rodents. R(-)-Deprenyl, a selective monoamine oxidase (MAO)-B inhibitor, has been shown to be capable of protecting animals against this DSP-4-induced neuronal degeneration. Its action, however, has been claimed to be unrelated to the inhibition of MAO-B activity but rather due to competition for the NA uptake sites. The effects of several types of MAO inhibitors against DSP-4 toxicity, MAO-B activity both in vivo and in vitro, and NA uptake into the hippocampus have been assessed. N-(2-Hexyl) N-methylpropargylamine (2-HxMP), a potent MAO-B inhibitor, for example, exerts no appreciable effect on NA uptake but is quite potent in counteracting the NA-depleting effect of DSP-4. Such results rule out the possibility that the neuroprotective effect of the MAO-B inhibitors is due mainly to their effect on NA uptake. The in vitro inhibition of MAO-B activity seems to correlate positively with their neuroprotective effects against DSP-4. In comparison to the MAO-B inhibitors, NA uptake blockers, such as desipramine and S(+)-deprenyl, exhibit relatively low efficacy in protecting the NA axon terminals from the effects of DSP-4-induced damage. The restoration of hippocampal NA levels is significantly enhanced with repeated treatments of R(-)-deprenyl or 2-HxMP even at very low doses following the DSP-4 insult. This suggests that in addition to neuroprotection, these MAO-B inhibitors may rescue some of the noradrenergic axon terminals damaged by DSP-4.

=&gt; FIL STNGUIDE

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LAST RELOADED: May 28, 2004 (20040528/UP).

=&gt;

3185

=> fil lreg

FILE 'LREGISTRY' ENTERED AT 08:45:30 ON 03 JUN 2004  
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STRUCTURE FILE UPDATES: 2 JUN 2004 HIGHEST RN 688737-01-1  
DICTIONARY FILE UPDATES: 2 JUN 2004 HIGHEST RN 688737-01-1

TSKA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

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Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more  
information enter HELP PROP at an arrow prompt in the file or refer  
to the file summary sheet on the web at:  
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=> fil hcaplus

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FILE COVERS 1907 - 3 Jun 2004 VOL 140 ISS 23  
FILE LAST UPDATED: 2 Jun 2004 (20040602/ED)

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=> fil zcaplus

FILE 'ZCAPLUS' ENTERED AT 08:45:44 ON 03 JUN 2004  
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FILE COVERS 1907 - 3 Jun 2004 VOL 140 ISS 23  
 FILE LAST UPDATED: 2 Jun 2004 (20040602/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

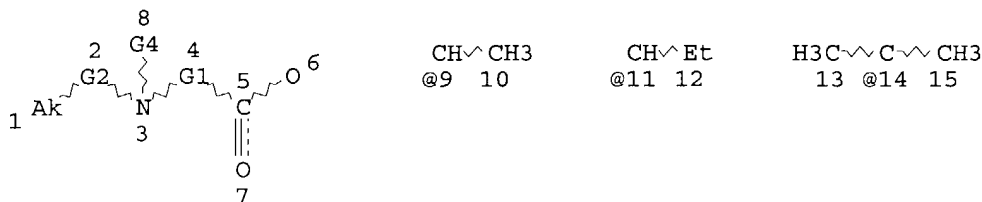
=> FIL STNGUIDE

FILE 'STNGUIDE' ENTERED AT 08:45:48 ON 03 JUN 2004  
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FILE CONTAINS CURRENT INFORMATION.  
 LAST RELOADED: May 28, 2004 (20040528/UP).

=> d que 196

L39 ( 1)SEA FILE=HCAPLUS ABB=ON PLU=ON (DURDEN, D? AND DAVIS, B? AND  
 DYCK,L? AND LIU, Y? AND BOULTON, A? AND PATERSON, I?)/AU  
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 L41 ( 103)SEA FILE=REGISTRY ABB=ON PLU=ON L40  
 L42 SCR 1518  
 L43 SCR 2050 2052 2043  
 L44 SCR 1526  
 L45 SCR 1235  
 L46 STR



H3C~C~Et  
 16 @17 18

REP G1=(1-3) CH2  
 VAR G2=CH2/9/11/14/17

VAR G4=H/CH3

NODE ATTRIBUTES:

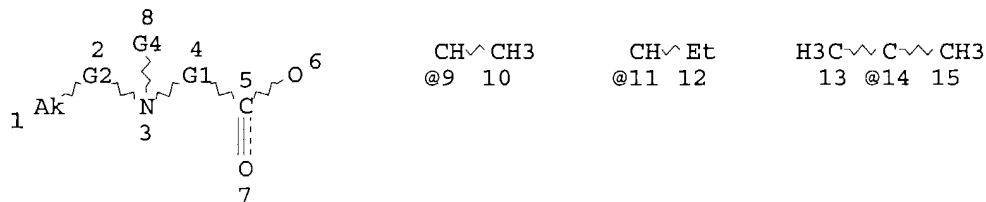
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CONNECT IS E1 RC AT 6  
DEFAULT MLEVEL IS ATOM  
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED  
NUMBER OF NODES IS 18

STEREO ATTRIBUTES: NONE

L47 SCR 963  
L48 ( 3584468)SEA FILE=REGISTRY ABB=ON PLU=ON N=1 NOT ((P/ELS OR SI/ELS)  
OR (TIS OR MNS OR AYS OR PMS)/CI OR SEQUENCE/FS)  
L49 ( 526)SEA FILE=REGISTRY SUB=L48 SSS FUL ((L42 AND L44 AND L45 AND  
L47) NOT L43) AND L46  
L50 ( 37)SEA FILE=REGISTRY ABB=ON PLU=ON L41 NOT (?NITRILE? OR  
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L51 ( 2)SEA FILE=REGISTRY ABB=ON PLU=ON L49 AND (C6 H13 N O2)/MF AND  
(?GLYCINE? AND ?METHYLETHYL? AND ?METHYL?)/CNS  
L52 ( 39)SEA FILE=REGISTRY ABB=ON PLU=ON L51 OR L50  
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OR 244190-02-1/CRN OR 244190-03-2/CRN OR 244190-04-3/CRN OR  
27453-30-1/CRN OR 31044-47-0/CRN OR 3183-21-9/CRN OR 3183-22-0/  
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L54 ( 41)SEA FILE=REGISTRY ABB=ON PLU=ON L52 OR L53  
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L56 ( 14)SEA FILE=HCAPLUS ABB=ON PLU=ON L55 AND (PY<1999 OR AY<1999  
OR PRY<1999)  
L57 3 SEA FILE=HCAPLUS ABB=ON PLU=ON L56 NOT (PESTICIDE? OR  
PHOTOGRAPHIC? OR FOSSIL? OR INK? OR ALLOY? OR UNIT? OR  
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L58 ( 1)SEA FILE=HCAPLUS ABB=ON PLU=ON (DURDEN, D? AND DAVIS, B? AND  
DYCK, L? AND LIU, Y? AND BOULTON, A? AND PATERSON, I?)/AU  
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L61 SCR 1518  
L62 SCR 2050 2052 2043  
L63 SCR 1526  
L64 SCR 1235  
L65 STR



H3C<sup>~</sup>C<sup>~</sup>Et  
16 @17 18

REP G1=(1-3) CH2  
VAR G2=CH2/9/11/14/17  
VAR G4=H/CH3



## NODE ATTRIBUTES:

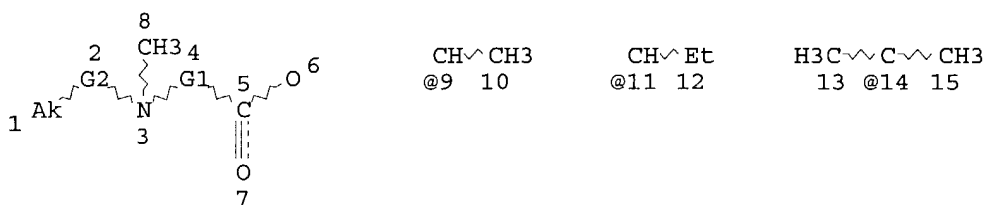
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 CONNECT IS E1 RC AT 6  
 DEFAULT MLEVEL IS ATOM  
 DEFAULT ECLEVEL IS LIMITED

## GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED  
 NUMBER OF NODES IS 18

## STEREO ATTRIBUTES: NONE

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 L67 ( 3584468)SEA FILE=REGISTRY ABB=ON PLU=ON N=1 NOT ((P/ELS OR SI/ELS)  
 OR (TIS OR MNS OR AYS OR PMS)/CI OR SEQUENCE/FS)  
 L68 ( 526)SEA FILE=REGISTRY SUB=L67 SSS FUL ((L61 AND L63 AND L64 AND  
 L66) NOT L62) AND L65  
 L69 ( 37)SEA FILE=REGISTRY ABB=ON PLU=ON L60 NOT (?NITRILE? OR  
 ?PHOSPHONIC? OR ?AMINE? OR ?PROPENOIC? OR ?BROMO?)/CNS  
 L70 ( 2)SEA FILE=REGISTRY ABB=ON PLU=ON L68 AND (C6 H13 N O2)/MF AND  
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 L71 ( 39)SEA FILE=REGISTRY ABB=ON PLU=ON L70 OR L69  
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 L73 ( 41)SEA FILE=REGISTRY ABB=ON PLU=ON L71 OR L72  
 L74 ( 18)SEA FILE=HCAPLUS ABB=ON PLU=ON L73 (L) (BIOL OR USES)/RL  
 L75 ( 14)SEA FILE=HCAPLUS ABB=ON PLU=ON L74 AND (PY<1999 OR AY<1999  
 OR PRY<1999)  
 L76 ( 3)SEA FILE=HCAPLUS ABB=ON PLU=ON L75 NOT (PESTICIDE? OR  
 PHOTOGRAPHIC? OR FOSSIL? OR INK? OR ALLOY? OR UNIT? OR  
 NONCONDENSED?)/SC  
 L77 ( 4)SEA FILE=HCAPLUS ABB=ON PLU=ON L74 NOT L75  
 L78 STR



H3C $\sim$ C $\sim$ Et  
 16 @17 18

REP G1=(1-3) CH2

VAR G2=CH2/9/11/14/17

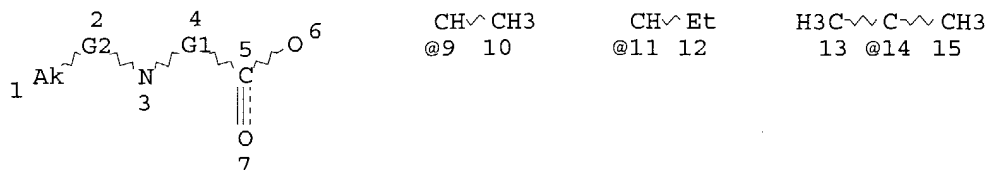
## NODE ATTRIBUTES:

CONNECT IS E1 RC AT 1  
 CONNECT IS E3 RC AT 3  
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 DEFAULT MLEVEL IS ATOM  
 DEFAULT ECLEVEL IS LIMITED  
 ECOUNT IS M1-X17 C AT 1

## GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED  
NUMBER OF NODES IS 18

STEREO ATTRIBUTES: NONE  
L79 STR



H3C $\sim$ C $\sim$ Et  
16 @17 18

REP G1=(1-3) CH2  
VAR G2=CH2/9/11/14/17  
NODE ATTRIBUTES:  
CONNECT IS E1 RC AT 1  
CONNECT IS E2 RC AT 3  
CONNECT IS E1 RC AT 6  
DEFAULT MLEVEL IS ATOM  
DEFAULT ECLEVEL IS LIMITED  
ECOUNT IS M1-X17 C AT 1

GRAPH ATTRIBUTES:  
RING(S) ARE ISOLATED OR EMBEDDED  
NUMBER OF NODES IS 17

STEREO ATTRIBUTES: NONE

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L82 ( 480)SEA FILE=HCAPLUS ABB=ON PLU=ON L81 AND (PY<1999 OR AY<1999  
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L84 ( 67)SEA FILE=HCAPLUS ABB=ON PLU=ON L83 AND US/PC.B  
L85 ( 25)SEA FILE=HCAPLUS ABB=ON PLU=ON L84 NOT (UNIT? OR LEATHER? OR  
DETERGENT? OR PHOTOGRAPHIC? OR FOSSIL? OR INK? OR ALLOY? OR  
EXPLOSIVE? OR PESTICID? OR WOOD? OR PETROLEUM? OR INORGANIC?  
OR PLASTIC?)/SC  
L86 ( 25)SEA FILE=HCAPLUS ABB=ON PLU=ON L85 NOT ((L76 OR L77))  
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L90 12 SEA FILE=HCAPLUS ABB=ON PLU=ON L89 NOT L76  
L91 1 SEA FILE=REGISTRY ABB=ON PLU=ON 7631-98-3/RN  
L92 228 SEA FILE=HCAPLUS ABB=ON PLU=ON L91  
L93 4 SEA FILE=HCAPLUS ABB=ON PLU=ON L90 NOT L92  
L94 8 SEA FILE=HCAPLUS ABB=ON PLU=ON L90 NOT L93  
L95 3 SEA FILE=HCAPLUS ABB=ON PLU=ON L94 AND (A61K?)/ICM  
L96 10 SEA FILE=HCAPLUS ABB=ON PLU=ON L93 OR L57 OR L95

=> d his 197

FILE 'HCAPLUS' ENTERED AT 08:07:49 ON 03 JUN 2004  
L97 8 S L96 NOT L38

=> d l97 ibib hitstr abs  
YOU HAVE REQUESTED DATA FROM FILE 'HCAPLUS' - CONTINUE? (Y)/N:y

L97 ANSWER 1 OF 8 HCAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 2003:435212 HCAPLUS  
DOCUMENT NUMBER: 139:3248  
TITLE: Betaines as adjuvants to susceptibility testing and  
antimicrobial therapy  
INVENTOR(S): Thornton, Charles G.  
PATENT ASSIGNEE(S): USA  
SOURCE: U.S. Pat. Appl. Publ., 103 pp., Cont.-in-part of U.S.  
6,406,880.  
CODEN: USXXCO  
DOCUMENT TYPE: **Patent**  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 2  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2003104513	A1	20030605	US 2002-125647	20020419 <--
WO 9850576	A1	19981112	WO 1998-US8760	19980501 <--
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
US 6406880	B1	20020618	US 1999-429614	19991029 <--
PRIORITY APPLN. INFO.:			US 1997-45512P	P 19970502 <--
			WO 1998-US8760	A1 19980501 <--
			US 1999-429614	A2 19991029
IT	<b>1462-54-0</b>			
	RL: BSU (Biological study, unclassified); BUU (Biological use, unclassified); THU (Therapeutic use); <b>BIOL (Biological study);</b> <b>USES (Uses)</b> (betaines as adjuvants to susceptibility testing and antimicrobial therapy)			
RN	1462-54-0 HCAPLUS			
CN	$\beta$ -Alanine, N-dodecyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)			

Me-(CH<sub>2</sub>)<sub>11</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-CO<sub>2</sub>H

AB The present invention is related to methods and compns. for susceptibility testing of bacteria containing mycolic acid structures using betaine-like detergents, and inducing the susceptibility of such bacteria using the same.

=> d 197 ibib hitstr abs 2-

YOU HAVE REQUESTED DATA FROM FILE 'HCAPLUS' - CONTINUE? (Y)/N:y

YOU HAVE REQUESTED DATA FROM 7 ANSWERS - CONTINUE? Y/(N):y

L97 ANSWER 2 OF 8 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1999:733825 HCAPLUS

DOCUMENT NUMBER: 131:348769

TITLE: Compositions and methods for enzymatic decontamination of microbiological samples for analysis and culture

INVENTOR(S): Thornton, Charles G.; MacLellan, Kerry M.

PATENT ASSIGNEE(S): Integrated Research Technology, L.L.C., USA

SOURCE: U.S., 42 pp.

CODEN: USXXAM

DOCUMENT TYPE: **Patent**

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5985593	A	19991116	US 1997-943338	19971003 <--
PRIORITY APPLN. INFO.:			US 1996-28470P	P 19961011 <--
OTHER SOURCE(S): MARPAT 131:348769				
IT 1462-54-0, N-Dodecyl-β-alanine				
RL: BUU (Biological use, unclassified); BIOL (Biological study);				
<b>USES (Uses)</b>				
(detergents; compns. and methods for enzymic decontamination of microbiol. samples for anal. and culture)				
RN	1462-54-0 HCAPLUS			
CN	β-Alanine, N-dodecyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)			

Me-(CH<sub>2</sub>)<sub>11</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-CO<sub>2</sub>H

AB The present invention is related to a method for the enzymic decontamination of specimens as a means to control microbiol. contamination. The compns. and methods of the invention are especially useful to eliminate non-gram neg. contaminants of samples being processed for microbiol. anal. Respiratory specimens were processed and treated with N-(3-carboxypropyl)-N,N-dimethyl-1-octadecanaminium, inner salt and with enzyme cocktail containing lysozyme, zymolyase, Trichoderma harzianum extract, and Cytophaga extract

REFERENCE COUNT: 71 THERE ARE 71 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L97 ANSWER 3 OF 8 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1993:588589 HCAPLUS

DOCUMENT NUMBER: 119:188589

TITLE: Antiviral composition and method

INVENTOR(S): Pollock, Jerry J.; Docherty, John J.

PATENT ASSIGNEE(S): Northeastern Ohio Universities College of Medicine, USA

SOURCE: U.S., 8 pp. Cont.-in-part of U.S. 5,185,153.

CODEN: USXXAM

DOCUMENT TYPE: **Patent**

LANGUAGE: English

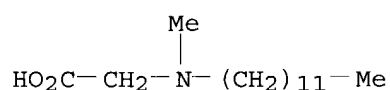
FAMILY ACC. NUM. COUNT: 2

## PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5213803	A	19930525	US 1992-840321	19920224 <--
US 5185153	A	19930209	US 1990-592552	19901004 <--
US 5270032	A	19931214	US 1992-925902	19920806 <--
PRIORITY APPLN. INFO.:			US 1990-592552	19901004 <--
			US 1991-671457	19910319 <--

IT 7631-98-3  
 RL: BIOL (Biological study)  
 (envelope virus-inhibiting pharmaceuticals containing)

RN 7631-98-3 HCAPLUS  
 CN Glycine, N-dodecyl-N-methyl-, sodium salt (9CI) (CA INDEX NAME)



● Na

AB A method for killing envelope viruses in vitro causing AIDS and herpes infections comprises contacting an infected surface or cavity with an antiviral formulation containing humectant (e.g. sorbitol, glycerol, etc.) 20-80%, and activating agents including inorg. monovalent anions and detergent with carrier or dispenser. The humectant facilitates structural and/or functional 3-dimensional disruption or disorientation of the viral envelope. Various combinations of ingredients in a mouthrinse were tested against herpes simplex virus (HSV)-1. The most potent antiviral activity (>99.9% inhibition) was only seen with all 5 ingredients (sorbitol, Tween 20, NaHCO<sub>3</sub>, NaSCN, and EtOH) together.

L97 ANSWER 4 OF 8 HCAPLUS COPYRIGHT 2004 ACS on STN

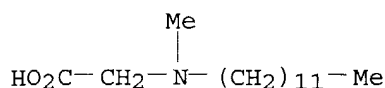
ACCESSION NUMBER: 1991:512653 HCAPLUS  
 DOCUMENT NUMBER: 115:112653  
 TITLE: Selective modification of the catalytic subunit of pertussis toxin  
 INVENTOR(S): Kaslow, Harvey R.  
 PATENT ASSIGNEE(S): USA  
 SOURCE: U.S., 10 pp.  
 CODEN: USXXAM  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5032398	A	19910716	US 1986-893080	19860801 <--
US 5165927	A	19921124	US 1991-682773	19910409 <--
PRIORITY APPLN. INFO.:			US 1986-893080	19860801 <--

IT 7631-98-3, Sodium lauryl sarcosine  
 RL: BIOL (Biological study)  
 (pertussis toxin activation response to, toxin selective alkylation and deactivation in relation to)

RN 7631-98-3 HCAPLUS

CN Glycine, N-dodecyl-N-methyl-, sodium salt (9CI) (CA INDEX NAME)



● Na

AB Pertussis toxin is selectively modified by deactivating key amino acids in the catalytic portion of the toxin, yet leaving the antigenic determinants on the  $\beta$ -oligomer essentially undisturbed. The process involves (1) activating the catalytic subunit with a mixture containing polyphosphate, a sulfhydryl reductant, and a mild detergent; and (2) alkylating the revealed SH groups. Pertussis toxin was incubated with DTT, CHAPS, and ATP for activation and then was alkylated with iodoacetate. The modified toxin gave a 3% NADase activity (untreated was 100%).

L97 ANSWER 5 OF 8 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1991:129164 HCAPLUS  
 DOCUMENT NUMBER: 114:129164  
 TITLE: Surfactant-based dry granular nonalcoholic oral drug delivery systems  
 INVENTOR(S): Wilson, Mark E.; Cole, B. Harrison  
 PATENT ASSIGNEE(S): Spectrum Consumer Products Co., Inc., USA  
 SOURCE: U.S., 6 pp. Cont.-in-part of U.S. 4,919,918.  
 CODEN: USXXAM  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 2  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4971785	A	19901120	US 1990-502618	19900330 <--
US 4919918	A	19900424	US 1988-167504	19880314 <--
CA 1328818	A1	19940426	CA 1989-593151	19890308 <--
AU 8931255	A1	19890914	AU 1989-31255	19890313 <--
JP 01275521	A2	19891106	JP 1989-63424	19890314 <--
JP 2938884	B2	19990825		
CA 2031572	AA	19911001	CA 1990-2031572	19901205 <--
CA 2031572	C	19960130		
EP 448895	A1	19911002	EP 1990-403685	19901219 <--
EP 448895	B1	19940525		
R: AT, BE, CH, DE, ES, FR, GB, IT, LI, LU, NL				
AT 106012	E	19940615	AT 1990-403685	19901219 <--
JP 05017345	A2	19930126	JP 1991-49707	19910314 <--
AU 9173693	A1	19910613	AU 1991-73693	19910321 <--
AU 635826	B2	19930401		
PRIORITY APPLN. INFO.:			US 1988-167504	19880314 <--
			US 1990-502618	19900330 <--
			EP 1990-403685	19901219 <--

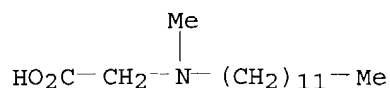
IT 7631-98-3, Sodium laurylsarcosinate

RL: BIOL (Biological study)

(oral drug formulations containing, granular)

RN 7631-98-3 HCAPLUS

CN Glycine, N-dodecyl-N-methyl-, sodium salt (9CI) (CA INDEX NAME)



● Na

AB The compns. comprise surfactants, such as Na laurylsulfate, Na laurylsarcosinate, Na alkylsulfoacetate, etc., spray-dried essential oils, and effervescence-causing components. A composition comprised aspirin 225, surfactant 5, sweetener 95, spray-dried essential oil 400, and effervescence-causing mixture 525 mg. A mouthwash can also be produced by this method.

L97 ANSWER 6 OF 8 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1989:552636 HCAPLUS

DOCUMENT NUMBER: 111:152636

TITLE: Amino acid derivatives as animal growth promoters

INVENTOR(S): Bauwe, Reinhard; Von Rottkay, Fritjof; Schwarz, Justus

PATENT ASSIGNEE(S): VEB Berlin-Chemie, Ger. Dem. Rep.

SOURCE: Ger. (East), 3 pp.

CODEN: GEXXA8

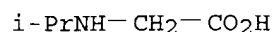
DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

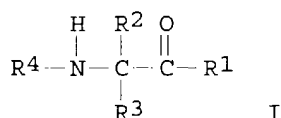
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DD 256073	A1	19880427	DD 1985-282385	19851104 <--
PRIORITY APPLN. INFO.:			DD 1985-282385	19851104 <--
OTHER SOURCE(S): MARPAT 111:152636				
IT 3338-22-5, N-Isopropylglycine hydrochloride				
RL: AGR (Agricultural use); BIOL (Biological study); USES				
(Uses)				
(feeding experiment with, on male rats)				
RN	3338-22-5 HCAPLUS			
CN	Glycine, N-(1-methylethyl)-, hydrochloride (9CI) (CA INDEX NAME)			



● HCl

GI



AB Amino acid derivs. I (R1 = OH, NH2, alkoxy, arylamino, alkylamino, dialkylamino; R2, R3 = H, lower alkyl; R4 = C1-5 alkyl) promote growth and feed utilization efficiency when added to animal feed or drinking water, or when applied to the animals mucous membranes. Growing male rats given water ad libitum containing 10 ppm N-isopropylglycine hydrochloride displayed a comparable feed utilization efficiency to those given drinking water containing ambagon/pseudothymine.

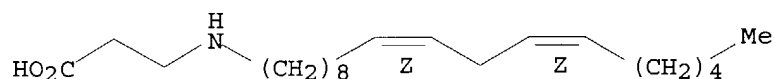
L97 ANSWER 7 OF 8 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1981:71506 HCAPLUS  
DOCUMENT NUMBER: 94:71506  
TITLE: Antiseptic composition for topical application to the skin for use against bromidrosis  
INVENTOR(S): Marcadet, Ernest  
PATENT ASSIGNEE(S): USA  
SOURCE: U.S., 9 pp. Cont. of U.S. Ser. No. 778,358, abandoned.  
CODEN: USXXAM  
DOCUMENT TYPE: **Patent**  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4224319	A	19800923	US 1979-62409	19790731 <--
PRIORITY APPLN. INFO.:			US 1973-374266	19730627 <--
			US 1974-500372	19740826 <--
			US 1975-622051	19751114 <--
			US 1977-778358	19770317 <--

IT 76382-07-5  
RL: **BIOL (Biological study)**  
(antiseptic composition containing, for bromidrosis treatment)  
RN 76382-07-5 HCAPLUS  
CN  $\beta$ -Alanine, N-9,12-octadecadienyl-, (Z,Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



AB An aqueous disinfectant composition, harmless to the skin, contains as the main active agent an amino acid RNH(R1NH)nR2CO2H (R = C8-18 aliphatic; R1 and R2 = C1-3 alkylene; n = 1 or 2), 1 or several triglycerides, and vitamins. Thus, an emulsion was formulated with alkylaminopropionic acid 1.95 g, oleic triglyceride [122-32-7] 6 g, and axerophthol palmitate [79-81-2] 0.6 mg.

L97 ANSWER 8 OF 8 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1979:151785 HCAPLUS  
DOCUMENT NUMBER: 90:151785  
TITLE: Fungicidal phenylnitramines  
INVENTOR(S): Cross, Barrington; Dawe, David H.  
PATENT ASSIGNEE(S): American Cyanamid Co., USA  
SOURCE: U.S., 17 pp.  
CODEN: USXXAM  
DOCUMENT TYPE: **Patent**  
LANGUAGE: English



FAMILY ACC. NUM. COUNT: 2

## PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4130645	A	19781219	US 1978-879340	19780221 <--
DE 2902890	A1	19790823	DE 1979-2902890	19790125 <--
AU 7944082	A1	19790830	AU 1979-44082	19790208 <--
BR 7900812	A	19790904	BR 1979-812	19790209 <--
EP 3881	A1	19790905	EP 1979-300201	19790209 <--
R: CH, FR, GB, IT, SE				
DD 143251	C	19800813	DD 1979-211101	19790219 <--
DK 7900729	A	19790822	DK 1979-729	19790220 <--
JP 54122233	A2	19790921	JP 1979-19616	19790221 <--
PRIORITY APPLN. INFO.:			US 1978-879340	19780221 <--

IT 69733-43-3P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation);

**USES (Uses)**

(preparation and fungicidal activity of)

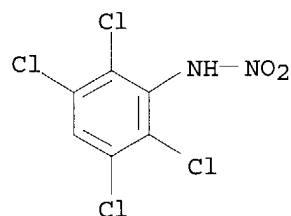
RN 69733-43-3 HCAPLUS

CN Butanoic acid, 4-(dodecylamino)-, compd. with 2,3,5,6-tetrachloro-N-nitrobenzenamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 54381-45-2

CMF C6 H2 Cl4 N2 O2



CM 2

CRN 41421-76-5

CMF C16 H33 N O2

$$\text{Me}-(\text{CH}_2)_{11}-\text{NH}-(\text{CH}_2)_3-\text{CO}_2\text{H}$$

AB Phenylnitramines  $\text{RnC}_6\text{H}_5\text{-nNR1NO}_2$  (I; R = the same or different halo, Me,  $\text{CF}_3$ ,  $\text{NO}_2$ , CN,  $\text{MeSO}_2$ , AcNH, etc.; R1 = H, alkyl, alkenyl, alkynyl,  $\text{PhCH}_2$ , haloalkyl, etc.) and 2,3,5,6-tetrachloro-N-nitroaniline salts  $2,3,5,6\text{-Cl}_4\text{C}_6\text{HN:N(O)O}^- \text{M}^+$  (II; M = Na, K, Ba/2, protonated amine,  $\text{NH}_4$ ,  $\text{Me}_4\text{N}$ ,  $\text{PhCH}_2\text{NEt}_3$ ), totalling 99, were prepared I (R1 = H) were prepared by nitration of anilines and were converted to I (R  $\neq$  H) by alkylation, acylation, etc., and II by treatment of 2,3,5,6- $\text{Cl}_4\text{C}_6\text{HNHNO}_2$  with amines or metal or quaternary ammonium salts. Both I and II showed good fungicidal activity.

=> FIL STNGUIDE

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FILE CONTAINS CURRENT INFORMATION.  
LAST RELOADED: May 28, 2004 (20040528/UP).

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=> fil lreg

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provided by InfoChem.

STRUCTURE FILE UPDATES: 2 JUN 2004 HIGHEST RN 688737-01-1  
DICTIONARY FILE UPDATES: 2 JUN 2004 HIGHEST RN 688737-01-1

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when  
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more  
information enter HELP PROP at an arrow prompt in the file or refer  
to the file summary sheet on the web at:  
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=> fil hcaplus

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FILE COVERS 1907 - 3 Jun 2004 VOL 140 ISS 23  
FILE LAST UPDATED: 2 Jun 2004 (20040602/ED)

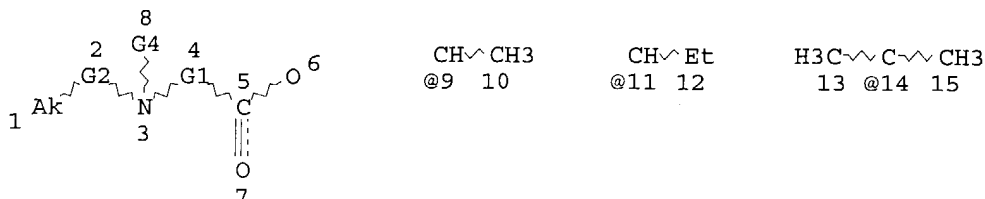
This file contains CAS Registry Numbers for easy and accurate  
substance identification.

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USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
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This file contains CAS Registry Numbers for easy and accurate substance identification.

$R_1 =$  unsubstituted alkyl group

compounds indexed  
for application



Page 2

REP G1=(1-3) CH2  
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 VAR G4=H/CH3  
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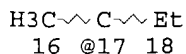
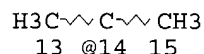
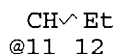
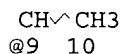
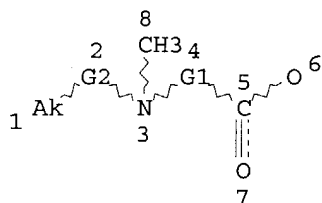
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STEREO ATTRIBUTES: NONE

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 OR (TIS OR MNS OR AYS OR PMS)/CI OR SEQUENCE/FS)  
 L11 ( 526)SEA FILE=REGISTRY SUB=L10 (SSS FUL) ((L4 AND L6 AND L7 AND L9)  
 NOT L5) AND L8  
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 OR 244190-02-1/CRN OR 244190-03-2/CRN OR 244190-04-3/CRN OR  
 27453-30-1/CRN OR 31044-47-0/CRN OR 3183-21-9/CRN OR 3183-22-0/  
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 L16 ( 41)SEA FILE=REGISTRY ABB=ON PLU=ON L14 OR L15  
 L17 STR

*set contains compounds  
 named in  
 application*



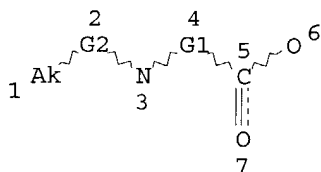
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 DEFAULT ECLEVEL IS LIMITED  
 ECOUNT IS M1-X17 C AT 1

GRAPH ATTRIBUTES:  
 RING(S) ARE ISOLATED OR EMBEDDED  
 NUMBER OF NODES IS 18

STEREO ATTRIBUTES: NONE

L18

STR

CH $\sim$ CH<sub>3</sub>  
@9 10CH $\sim$ Et  
@11 12H<sub>3</sub>C $\sim$ C $\sim$ CH<sub>3</sub>  
13 @14 15H<sub>3</sub>C $\sim$ C $\sim$ Et  
16 @17 18

REP G1=(1-3) CH2  
 VAR G2=CH2/9/11/14/17  
 NODE ATTRIBUTES:  
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 CONNECT IS E2 RC AT 3  
 CONNECT IS E1 RC AT 6  
 DEFAULT MLEVEL IS ATOM  
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STEREO ATTRIBUTES: NONE

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 L21 ( 5)SEA FILE=REGISTRY ABB=ON PLU=ON (58482-93-2 OR 42313-51-9 OR 3338-22-5 OR 3183-22-0 OR 3183-21-9)/RN  
 L22 ( 36)SEA FILE=REGISTRY ABB=ON PLU=ON L16 NOT L21  
 L23 ( 34)SEA FILE=HCAPLUS ABB=ON PLU=ON L22  
 L24 ( 28)SEA FILE=HCAPLUS ABB=ON PLU=ON L23 AND (PY<1999 OR AY<1999 OR PRY<1999)  
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 L29 28 SEA FILE=HCAPLUS ABB=ON PLU=ON L27 OR L28  
 L32 5 SEA FILE=HCAPLUS ABB=ON PLU=ON (58482-93-2? OR 42313-51-9?) (L) (BIOL OR USES)/RL  
 L33 5 SEA FILE=HCAPLUS ABB=ON PLU=ON L32 AND (PY<1999 OR AY<1999 OR PRY<1999)  
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 L35 14 SEA FILE=HCAPLUS ABB=ON PLU=ON L34 AND (PY<1999 OR AY<1999 OR PRY<1999)  
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 L38 33 SEA FILE=HCAPLUS ABB=ON PLU=ON L37 OR L33 OR L29

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YOU HAVE REQUESTED DATA FROM FILE 'HCAPLUS' - CONTINUE? (Y)/N:y

L38 ANSWER 1 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1999:626163 HCAPLUS  
 DOCUMENT NUMBER: 131:243589  
 TITLE: Aliphatic amino carboxylic and amino phosphonic acids, amino nitriles, and amino tetrazoles as cellular rescue agents  
 INVENTOR(S): Paterson, I. Alick; Dyck, Lilian E.; Davis, Bruce A.; Liu, Ya-Dong; Durden, David A.; Boulton, Alan A.  
 PATENT ASSIGNEE(S): University of Saskatchewan Technologies Inc., Can.; The Canada Trust Company  
 SOURCE: PCT Int. Appl., 52 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9948858	A2	19990930	WO 1999-CA250	19990325 <--
WO 9948858	A3	20000120		
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
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AU 9928240	A1	19991018	AU 1999-28240	19990325 <--
AU 767098	B2	20031030		
TR 200002756	T2	20001221	TR 2000-200002756	19990325 <--
EP 1064254	A2	20010103	EP 1999-908728	19990325 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
BR 9909103	A	20011016	BR 1999-9103	19990325 <--
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ZA 2000004988	A	20010507	ZA 2000-4988	20000919 <--
NO 2000004774	A	20000925	NO 2000-4774	20000925 <--
PRIORITY APPLN. INFO.:			US 1998-79488P	P 19980326 <--
			US 1998-79489P	P 19980326 <--
			WO 1999-CA250	W 19990325

OTHER SOURCE(S): MARPAT 131:243589

IT 3338-22-5P 31044-48-1P 41331-11-7P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of aliphatic amino carboxylic and amino phosphonic acids, amino nitriles, and amino tetrazoles as cellular rescue agents)

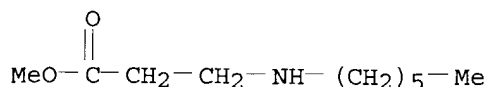
RN 3338-22-5 HCAPLUS

CN Glycine, N-(1-methylethyl)-, hydrochloride (9CI) (CA INDEX NAME)

i-PrNH-CH<sub>2</sub>-CO<sub>2</sub>H

● HCl

RN 31044-48-1 HCAPLUS  
CN β-Alanine, N-hexyl-, methyl ester, hydrochloride (8CI, 9CI) (CA INDEX NAME)



● HCl

RN 41331-11-7 HCAPLUS  
CN β-Alanine, N-hexyl- (9CI) (CA INDEX NAME)

Me-(CH<sub>2</sub>)<sub>5</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-CO<sub>2</sub>H

IT 3183-21-9P 3183-22-0P 3183-23-1P  
16217-35-9P 27453-30-1P 31044-47-0P  
40870-77-7P 41331-10-6P 42313-51-9P  
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244190-37-2P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);

**BIOL (Biological study); PREP (Preparation); USES (Uses)**

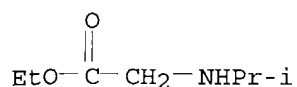
(preparation of aliphatic amino carboxylic and amino phosphonic acids, amino nitriles, and amino tetrazoles as cellular rescue agents)

RN 3183-21-9 HCAPLUS  
CN Glycine, N-(1-methylethyl)- (9CI) (CA INDEX NAME)

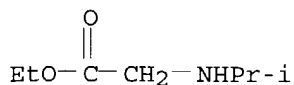
i-PrNH-CH<sub>2</sub>-CO<sub>2</sub>H

RN 3183-22-0 HCAPLUS  
CN Glycine, N-(1-methylethyl)-, ethyl ester (9CI) (CA INDEX NAME)



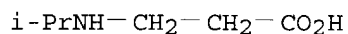


RN 3183-23-1 HCAPLUS  
 CN Glycine, N-(1-methylethyl)-, ethyl ester, hydrochloride (9CI) (CA INDEX NAME)

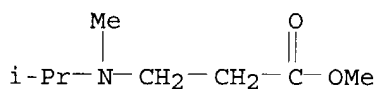


● HCl

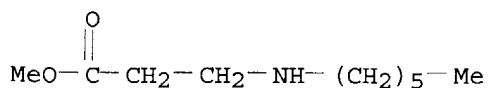
RN 16217-35-9 HCAPLUS  
 CN  $\beta$ -Alanine, N-(1-methylethyl)- (9CI) (CA INDEX NAME)



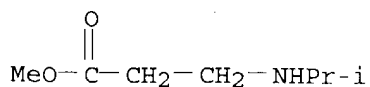
RN 27453-30-1 HCAPLUS  
 CN  $\beta$ -Alanine, N-methyl-N-(1-methylethyl)-, methyl ester (9CI) (CA INDEX NAME)



RN 31044-47-0 HCAPLUS  
 CN  $\beta$ -Alanine, N-hexyl-, methyl ester (8CI, 9CI) (CA INDEX NAME)

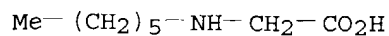


RN 40870-77-7 HCAPLUS  
 CN  $\beta$ -Alanine, N-(1-methylethyl)-, methyl ester, hydrochloride (9CI) (CA INDEX NAME)

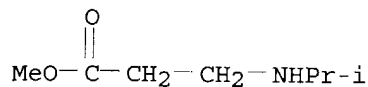


● HCl

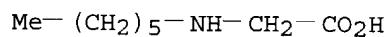
RN 41331-10-6 HCAPLUS  
 CN Glycine, N-hexyl- (9CI) (CA INDEX NAME)



RN 42313-51-9 HCAPLUS  
 CN  $\beta$ -Alanine, N-(1-methylethyl)-, methyl ester (9CI) (CA INDEX NAME)



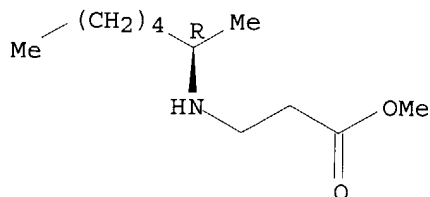
RN 56676-69-8 HCAPLUS  
 CN Glycine, N-hexyl-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 244189-67-1 HCAPLUS  
 CN  $\beta$ -Alanine, N-[(1R)-1-methylhexyl]-, methyl ester, hydrochloride (9CI)  
 (CA INDEX NAME)

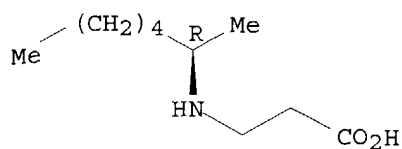
Absolute stereochemistry.



● HCl

RN 244189-68-2 HCAPLUS  
 CN  $\beta$ -Alanine, N-[(1R)-1-methylhexyl]-, hydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

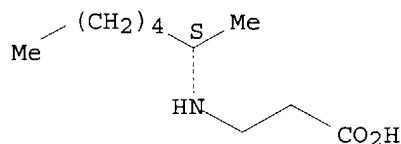


● HCl

RN 244189-69-3 HCAPLUS

CN β-Alanine, N-[(1S)-1-methylhexyl]-, hydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● HCl

RN 244189-70-6 HCAPLUS

CN β-Alanine, N-(1-methylethyl)-, hydrochloride (9CI) (CA INDEX NAME)

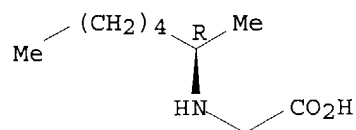
i-PrNH-CH<sub>2</sub>-CH<sub>2</sub>-CO<sub>2</sub>H

● HCl

RN 244189-71-7 HCAPLUS

CN Glycine, N-[(1R)-1-methylhexyl]-, hydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

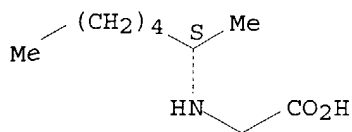


● HCl

RN 244189-72-8 HCAPLUS

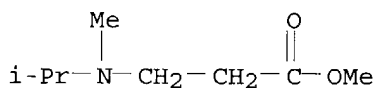
CN Glycine, N-[(1S)-1-methylhexyl]-, hydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● HCl

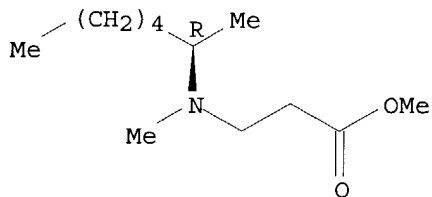
RN 244189-73-9 HCAPLUS  
 CN  $\beta$ -Alanine, N-methyl-N-(1-methylethyl)-, methyl ester, hydrochloride  
 (9CI) (CA INDEX NAME)



● HCl

RN 244189-74-0 HCAPLUS  
 CN  $\beta$ -Alanine, N-methyl-N-[(1R)-1-methylhexyl]-, methyl ester,  
 hydrochloride (9CI) (CA INDEX NAME)

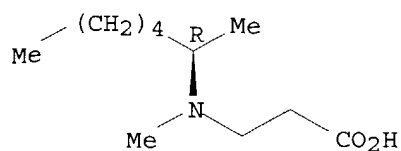
Absolute stereochemistry.



● HCl

RN 244189-75-1 HCAPLUS  
 CN  $\beta$ -Alanine, N-methyl-N-[(1R)-1-methylhexyl]-, hydrochloride (9CI) (CA  
 INDEX NAME)

Absolute stereochemistry.

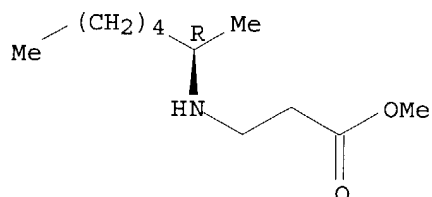


● HCl

RN 244189-98-8 HCAPLUS

CN β-Alanine, N-[(1R)-1-methylhexyl]-, methyl ester (9CI) (CA INDEX NAME)

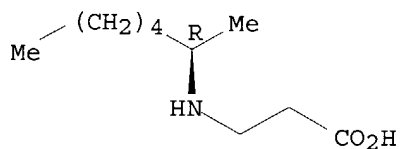
Absolute stereochemistry.



RN 244189-99-9 HCAPLUS

CN β-Alanine, N-[(1R)-1-methylhexyl]- (9CI) (CA INDEX NAME)

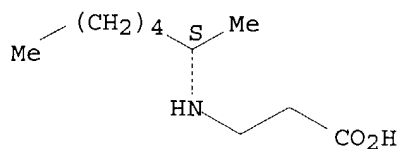
Absolute stereochemistry.



RN 244190-00-9 HCAPLUS

CN β-Alanine, N-[(1S)-1-methylhexyl]- (9CI) (CA INDEX NAME)

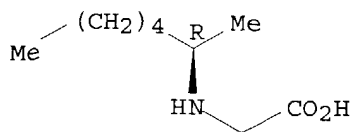
Absolute stereochemistry.



RN 244190-01-0 HCAPLUS

CN Glycine, N-[(1R)-1-methylhexyl]- (9CI) (CA INDEX NAME)

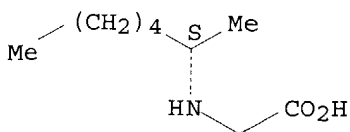
Absolute stereochemistry.



RN 244190-02-1 HCAPLUS

CN Glycine, N-[(1S)-1-methylhexyl]- (9CI) (CA INDEX NAME)

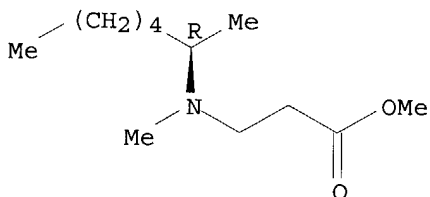
Absolute stereochemistry.



RN 244190-03-2 HCAPLUS

CN  $\beta$ -Alanine, N-methyl-N-[(1R)-1-methylhexyl]-, methyl ester (9CI) (CA INDEX NAME)

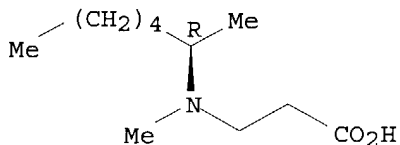
Absolute stereochemistry.



RN 244190-04-3 HCAPLUS

CN  $\beta$ -Alanine, N-methyl-N-[(1R)-1-methylhexyl]- (9CI) (CA INDEX NAME)

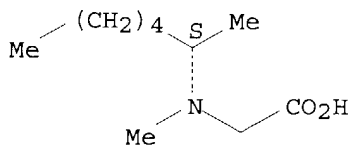
Absolute stereochemistry.



RN 244190-26-9 HCAPLUS

CN Glycine, N-methyl-N-[(1S)-1-methylhexyl]- (9CI) (CA INDEX NAME)

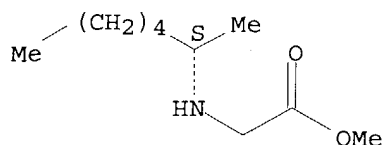
Absolute stereochemistry.



RN 244190-27-0 HCAPLUS

CN Glycine, N-[(1S)-1-methylhexyl]-, methyl ester (9CI) (CA INDEX NAME)

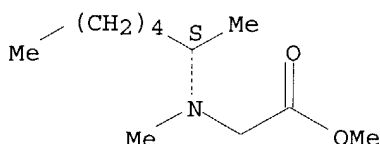
Absolute stereochemistry.



RN 244190-28-1 HCAPLUS

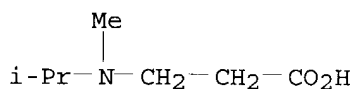
CN Glycine, N-methyl-N-[(1S)-1-methylhexyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



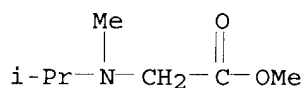
RN 244190-31-6 HCAPLUS

CN  $\beta$ -Alanine, N-methyl-N-(1-methylethyl)- (9CI) (CA INDEX NAME)



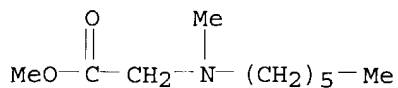
RN 244190-32-7 HCAPLUS

CN Glycine, N-methyl-N-(1-methylethyl)-, methyl ester (9CI) (CA INDEX NAME)



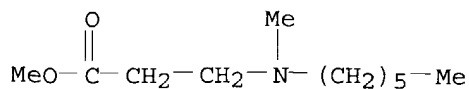
RN 244190-33-8 HCAPLUS

CN Glycine, N-hexyl-N-methyl-, methyl ester (9CI) (CA INDEX NAME)

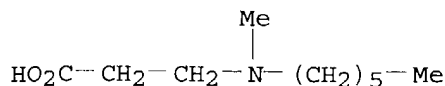


RN 244190-34-9 HCAPLUS

CN  $\beta$ -Alanine, N-hexyl-N-methyl-, methyl ester (9CI) (CA INDEX NAME)



RN 244190-37-2 HCAPLUS  
 CN  $\beta$ -Alanine, N-hexyl-N-methyl- (9CI) (CA INDEX NAME)

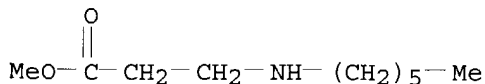


AB Title compds. R1R2R3CNR4(CH2)nX [R1 = Me(CH2)n (n = 1-16), alkenyl, alkynyl, alkoxy, alkylthio, alkylsulfinyl; R2 = H, Me, Et; R3, R4 = H, Me; X = CO2H or carbalkoxy, cyano, PO3H2 or phosphonate ester, 5-tetrazolyl] or their pharmaceutically acceptable salts were prepared. Thus, Me 3-(1-hexylamino)propionate hydrochloride was prepared by addition reaction of 1-hexylamine with Me acrylate and shown to have antiapoptotic activity at 10-6 M.

=> d l38 ibib hitstr abs 2-  
 YOU HAVE REQUESTED DATA FROM FILE 'HCAPLUS' - CONTINUE? (Y)/N:y

YOU HAVE REQUESTED DATA FROM 32 ANSWERS - CONTINUE? Y/(N):y

L38 ANSWER 2 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN  
 ACCESSION NUMBER: 1998:675926 HCAPLUS  
 DOCUMENT NUMBER: 130:3527  
 TITLE: Selective addition of amines to methyl acrylate in presence of alumina  
 AUTHOR(S): Suzuki, Yoshitada; Murakami, Shunsuke; Kodomari, Mitsuo  
 CORPORATE SOURCE: Department of Industrial Chemistry, Faculty of Engineering, Shibaura Institute of Technology, Minato-ku, Tokyo, 108-8548, Japan  
 SOURCE: Nippon Kagaku Kaishi (1998), (10), 664-669  
 CODEN: NKAKB8; ISSN: 0369-4577  
 PUBLISHER: Nippon Kagakkai  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Japanese  
 IT 31044-47-0P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (selective addition of amines to Me acrylate in presence of alumina)  
 RN 31044-47-0 HCAPLUS  
 CN  $\beta$ -Alanine, N-hexyl-, methyl ester (8CI, 9CI) (CA INDEX NAME)



AB The Michael type addition of primary amines to Me acrylate in benzene was accelerated by alumina, and monoadducts were selectively obtained in high yield. The reaction in benzene did not proceed without alumina. The yields of adducts were dependent on the structure of amines; the monoadducts were obtained in high yield (77-91% yield) when linear amines were used, and in the case of branched or bulky primary amines and secondary amines, the yields were decreased compared to the linear ones. In the addition of diamines to Me acrylate, only an amino group on 1 side of the diamines added to Me acrylate to give the monoadducts selectively, and



the amino group on the another side did not react. In the addition of asym. diamine, the less hindered amino group predominantly reacted with Me acrylate.

L38 ANSWER 3 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN  
 ACCESSION NUMBER: 1998:45464 HCAPLUS  
 DOCUMENT NUMBER: 128:128268  
 TITLE: Solid Phase Synthesis of  $\beta$ -Peptoids:  
 N-Substituted  $\beta$ -Aminopropionic Acid Oligomers  
 AUTHOR(S): Hamper, Bruce C.; Kolodziej, Stephen A.; Scates,  
 Angela M.; Smith, Ronald G.; Cortez, Enriqueta  
 CORPORATE SOURCE: Monsanto Company, St. Louis, MO, 63167, USA  
 SOURCE: Journal of Organic Chemistry (1998), 63(3),  
 708-718  
 CODEN: JOCEAH; ISSN: 0022-3263  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 IT 1462-54-0DP, N-Dodecyl- $\beta$ -alanine, ester with Wang resin  
 16217-35-9DP, ester with Wang resin 98430-14-9DP, ester  
 with Wang resin 202059-85-6DP, ester with Wang resin  
 202059-91-4DP, ester with Wang resin  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (solid-phase synthesis of substituted aminopropionic acid oligomers)  
 RN 1462-54-0 HCAPLUS  
 CN  $\beta$ -Alanine, N-dodecyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

Me- (CH<sub>2</sub>)<sub>11</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-CO<sub>2</sub>H

102 (b)

RN 16217-35-9 HCAPLUS  
 CN  $\beta$ -Alanine, N-(1-methylethyl)- (9CI) (CA INDEX NAME)

i-PrNH-CH<sub>2</sub>-CH<sub>2</sub>-CO<sub>2</sub>H

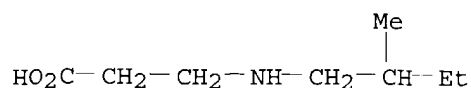
RN 98430-14-9 HCAPLUS  
 CN  $\beta$ -Alanine, N-(2-methylpropyl)- (9CI) (CA INDEX NAME)

i-BuNH-CH<sub>2</sub>-CH<sub>2</sub>-CO<sub>2</sub>H

RN 202059-85-6 HCAPLUS  
 CN  $\beta$ -Alanine, N-(1-methylpropyl)- (9CI) (CA INDEX NAME)

NH-CH<sub>2</sub>-CH<sub>2</sub>-CO<sub>2</sub>H  
 |  
 Me-CH-Et

RN 202059-91-4 HCAPLUS  
 CN  $\beta$ -Alanine, N-(2-methylbutyl)- (9CI) (CA INDEX NAME)



IT 202060-00-2P 202060-01-3P 202060-02-4P

202060-06-8P 202060-11-5P

RL: SPN (Synthetic preparation); PREP (Preparation)

(solid-phase synthesis of substituted aminopropionic acid oligomers)

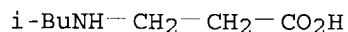
RN 202060-00-2 HCAPLUS

CN  $\beta$ -Alanine, N-(2-methylpropyl)-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 98430-14-9

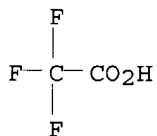
CMF C7 H15 N O2



CM 2

CRN 76-05-1

CMF C2 H F3 O2



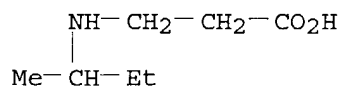
RN 202060-01-3 HCAPLUS

CN  $\beta$ -Alanine, N-(1-methylpropyl)-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 202059-85-6

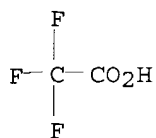
CMF C7 H15 N O2



CM 2

CRN 76-05-1

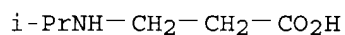
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RN 202060-02-4 HCAPLUS  
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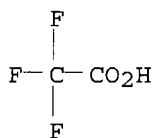
CM 1

CRN 16217-35-9  
 CMF C6 H13 N O2



CM 2

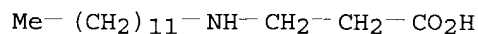
CRN 76-05-1  
 CMF C2 H F3 O2



RN 202060-06-8 HCAPLUS  
 CN  $\beta$ -Alanine, N-dodecyl-, trifluoroacetate (9CI) (CA INDEX NAME)

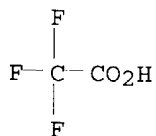
CM 1

CRN 1462-54-0  
 CMF C15 H31 N O2



CM 2

CRN 76-05-1  
 CMF C2 H F3 O2

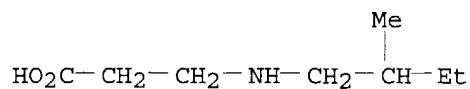


RN 202060-11-5 HCAPLUS  
 CN  $\beta$ -Alanine, N-(2-methylbutyl)-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 202059-91-4

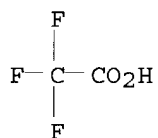
CMF C8 H17 N O2



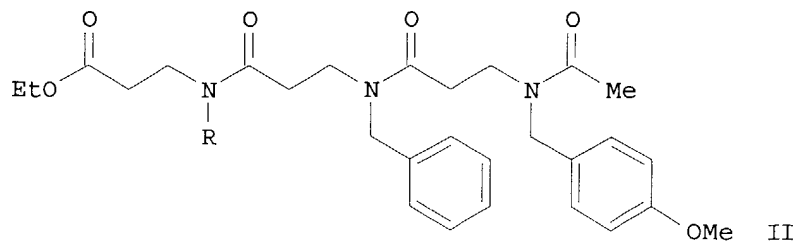
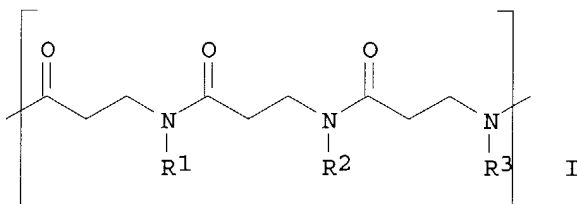
CM 2

CRN 76-05-1

CMF C2 H F3 O2



GI



AB A solid-phase organic synthesis method has been developed for the preparation  
 of

N-substituted- $\beta$ -aminopropionic acid oligomers or  $\beta$ -peptoids I.  
 Treatment of polymer-bound 4-(benzyloxy)benzyl acrylate with primary  
 amines afforded N-substituted  $\beta$ -alanines. Polymer loadings and

product conversions were determined by direct cleavage of resin-bound materials and measurement by <sup>1</sup>H NMR with an internal standard. The NMR method was used to establish loading of all resin-bound intermediates including acrylic acid. Acylation with acryloyl chloride followed by Michael addition of primary amines to the acrylamide allowed preparation of di-β-peptoids. By a linear set of seven reactions, trimeric N-benzyl-β-aminopropionic acid was prepared in 67% overall yield. Single-bead FT-IR microspectroscopy was used to acquire spectra of the resin bound mono-β-peptoids, di-β-peptoids, and acrylamide intermediates. A combinatorial library of defined mixts. of tri-β-peptoids was prepared by mixing equimolar amts. of the mono-β-peptoid resins and carrying them through two sequences of the acylation-Michael addition. The identity of a sample mixture II (R = Me, CH<sub>2</sub>Ph, CH<sub>2</sub>CH<sub>2</sub>Ph, CH<sub>2</sub>C<sub>6</sub>H<sub>4</sub>OMe-4, allyl, CH<sub>2</sub>CHMe<sub>2</sub>, CHMeEt, CHMe<sub>2</sub>) was determined by LC-MS anal. of the cleavage product.

REFERENCE COUNT: 66 THERE ARE 66 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L38 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1996:637648 HCAPLUS

DOCUMENT NUMBER: 126:24866

TITLE: Desensitizing solution for offset printing plate

INVENTOR(S): Itakura, Ryosuke; Kasai, Seishi; Sera, Hidefumi; Kato, Eiichi

PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd., Japan

SOURCE: U.S., 35 pp.  
CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5565290	A	19961015	US 1992-920862	19920728 <--
US 5723239	A	19980303	US 1996-718949	19960926 <--
			JP 1991-190081	19910730 <--
			JP 1991-269609	19911017 <--
			JP 1991-269917	19911018 <--
			JP 1991-269918	19911018 <--
			JP 1991-320488	19911204 <--
			US 1992-920862	19920728 <--

OTHER SOURCE(S): MARPAT 126:24866

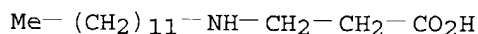
IT 1462-54-0 41331-11-7 101816-76-6

RL: TEM (Technical or engineered material use); USES (Uses)

(offset printing plate preparation by electrophotog. using desensitizing solns. containing phytic acid derivative and)

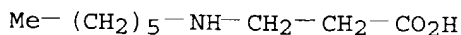
RN 1462-54-0 HCAPLUS

CN β-Alanine, N-dodecyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

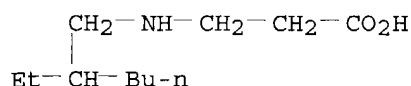


RN 41331-11-7 HCAPLUS

CN β-Alanine, N-hexyl- (9CI) (CA INDEX NAME)



RN 101816-76-6 HCAPLUS  
 CN  $\beta$ -Alanine, N-(2-ethylhexyl)- (9CI) (CA INDEX NAME)



AB An amine compound-containing, but cyanogen-free, desensitizing solution for an offset printing plate prepared from an electrophotog. material, characterized by containing phytic acid and/or a metal and/or ammonium salts of phytic acid and at least one imide compound containing 1-6 amino groups of formula -NR<sub>1</sub>R<sub>2</sub> and 1-6 imide bonds of the formula -CON(R<sub>3</sub>)CO- (R<sub>1</sub>, R<sub>2</sub> = H or an organic group or R<sub>1</sub> and R<sub>2</sub> together may form a cyclic structure; R<sub>3</sub> = H, halogen, cyano, nitro, or an organic group).

L38 ANSWER 5 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1995:878827 HCAPLUS

DOCUMENT NUMBER: 123:286739

TITLE: Preparation of N-alkylated amino acid and peptide chelating agents and their chelates with radionuclides.

INVENTOR(S): Spies, Hartmut; Schulze, Paul-Eberhard; Noll, Bernd; Noll, Steffi; Dinkelborg, Ludger

PATENT ASSIGNEE(S): Institut fuer Diagnostikforschung GmbH an der Freien Universitaet Berlin, Germany

SOURCE: Ger. Offen., 32 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 4337600	A1	19950504	DE 1993-4337600	19931101 <--
ZA 9408411	A	19950630	ZA 1994-8411	19941026 <--
WO 9512610	A1	19950511	WO 1994-DE1295	19941027 <--
W: AU, CA, CN, HU, JP, KR, NO, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
CA 2173844	AA	19950511	CA 1994-2173844	19941027 <--
AU 9481038	A1	19950523	AU 1994-81038	19941027 <--
AU 681919	B2	19970911		
EP 726909	A1	19960821	EP 1995-900059	19941027 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
CN 1134158	A	19961023	CN 1994-193990	19941027 <--
HU 74881	A2	19970228	HU 1996-1140	19941027 <--
JP 09508351	T2	19970826	JP 1994-512959	19941027 <--
NO 9601743	A	19960430	NO 1996-1743	19960430 <--
PRIORITY APPLN. INFO.:			DE 1993-4337600	19931101 <--
			WO 1994-DE1295	19941027 <--

OTHER SOURCE(S): MARPAT 123:286739

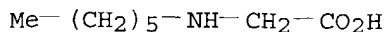
IT 41331-10-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of N-alkylated amino acid and peptide chelating agents and their chelates with radionuclides)

RN 41331-10-6 HCAPLUS

CN Glycine, N-hexyl- (9CI) (CA INDEX NAME)



AB R3SCH2CONR1(CH2CONH)nCH2COR2 [n = 0-2; R1 = (O-interrupted or O-substituted) alkyl, carboxyalkyl, hydroxyalkyl, aminoalkyl, etc., (substituted) Ph, cyclohexyl, etc.; R2 = halo, halomethyl, MeCO, NH2, OH, etc.; R3 = H, Ac, PhCO, acetamidomethyl, EtS, trityl, etc.], were prepared. Thus, glycine anhydride in aqueous NaOH was treated with ClCH2COCl at 0° to give ClCH2CO-Gly-Gly-OH, which was kept with hexylamine in EtOH to give Me(CH2)5-Gly-Gly-OH. The latter was stirred with ClCH2COCl in aqueous NaOH and the product was stirred with thiobenzoic acid in MeOH to give N-(benzoylmercaptoacetyl)-N-hexylglycylglycylglycine, which was hydrogenolyzed to give N-(mercaptoacetyl)-N-hexylglycylglycylglycine, the 99mTc complex of which was used to image atherosclerotic changes in rabbits.

L38 ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1995:777639 HCAPLUS

DOCUMENT NUMBER: 123:198616

TITLE: Preparation of N-sulfonylindoline derivatives with affinity for vasopressin and oxytocin receptors

INVENTOR(S): Wagnon, Jean; de Cointet, Paul; Nisato, Dino; Plouzane, Claude; Sereadeil-Legal, Claudine; Tonnerre, Bernard

PATENT ASSIGNEE(S): Elf Sanofi SA, Fr.

SOURCE: U.S., 50 pp. Cont.-in-part of U.S. Ser. No.737,655, abandoned.

CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5338755	A	19940816	US 1992-923839	19920803 <--
FR 2665441	A1	19920207	FR 1990-9778	19900731 <--
FR 2665441	B1	19921204		
IL 114934	A1	19960804	IL 1991-114934	19910730 <--
HU 219351	B	20010328	HU 1971-99045	19910731 <--
FR 2679903	A1	19930205	FR 1991-9908	19910802 <--
FR 2679903	B1	19931203		
AU 9224758	A1	19930302	AU 1992-24758	19920731 <--
AU 658664	B2	19950427		
BR 9205336	A	19931116	BR 1992-5336	19920731 <--
JP 06501960	T2	19940303	JP 1993-503337	19920731 <--
RU 2104268	C1	19980210	RU 1993-5168	19920731 <--
IL 117592	A1	19990411	IL 1992-117592	19920731 <--
CZ 288173	B6	20010516	CZ 1993-682	19920731 <--
CA 2206776	C	20020226	CA 1992-2206776	19920731 <--
SK 283463	B6	20030805	SK 1993-426	19920731 <--
NO 9301262	A	19930526	NO 1993-1262	19930401 <--
NO 180047	B	19961028		
NO 180047	C	19970205		
US 5397801	A	19950314	US 1994-240360	19940510 <--
US 5481005	A	19960102	US 1994-348150	19941128 <--
US 5578633	A	19961126	US 1995-458614	19950602 <--
FI 9800175	A	19980127	FI 1998-175	19980127 <--

## PRIORITY APPLN. INFO.:

FR 1990-9778	A 19900731 <--
US 1991-737655	B2 19910730 <--
FR 1991-9908	A 19910802 <--
IL 1991-99012	A3 19910730 <--
HU 1991-2552	A 19910731 <--
CA 1992-2093221	A3 19920731 <--
CS 1993-682	A 19920731 <--
IL 1992-102703	A3 19920731 <--
WO 1992-FR758	A 19920731 <--
US 1992-923839	A3 19920803 <--
FI 1993-1476	A 19930401 <--
US 1993-923839	A3 19930803 <--
US 1994-240360	A3 19940510 <--
US 1994-348150	A3 19941128 <--

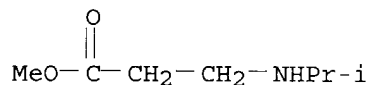
OTHER SOURCE(S): MARPAT 123:198616

IT 42313-51-9P

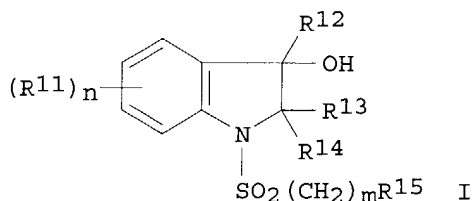
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of N-sulfonylindoline derivs. with affinity for vasopressin and oxytocin receptors)

RN 42313-51-9 HCAPLUS

CN  $\beta$ -Alanine, N-(1-methylethyl)-, methyl ester (9CI) (CA INDEX NAME)

GI



AB Title compds. I ( $R'1$  = halo, C1-4 alkyl, HO, C1-4 alkoxy,  $\text{PhCH}_2\text{O}$ , NC,  $\text{F}_3\text{C}$ ,  $\text{O}_2\text{N}$ ,  $\text{H}_2\text{N}$ ;  $R'2$  = C1-6 alkyl, C3-7 cycloalkyl, C5-7 cycloalkylene, (substituted) Ph, etc.;  $R'3$  = H;  $R'4$  =  $\text{H}_2\text{NCO}$ ,  $R'6R'7\text{NCO}$  wherein  $R'6R'7\text{N}$  = saturated 5-membered substituted N-heterocyclyl;  $R'5$  = C1-4 alkyl, 1-, 2-naphthyl, (substituted) Ph, etc.;  $n = m = 0-2$ ) or a salt thereof, are prepared  $\text{CH}_2\text{BrCONMe}_2$  (preparation given) and 5-chloro-2-(tosylamino)phenyl cyclohexyl ketone were reacted to give 2-[N-tosyl-N-(dimethylcarbamoylmethyl)amino]-5-(chlorophenyl) cyclohexyl ketone which in THF was treated with Li diisopropylamide to give after workup trans-I ( $R'1n$  = 5-Cl,  $R'2$  = cyclohexyl,  $R'3$  = H,  $R'4$  =  $\text{Me}_2\text{NCO}$ ,  $R'5$  = 4-MeC<sub>6</sub>H<sub>4</sub>,  $m = 0$ ). The IC<sub>50</sub> of I affinity for oxytocin receptors was 10<sup>-5</sup>-10<sup>-8</sup>M.

L38 ANSWER 7 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1993:46312 HCAPLUS

DOCUMENT NUMBER: 118:46312

TITLE: Solubilization of copper(II) complexes of N-alkyl- $\beta$ -alanines in their micellar solutions



AUTHOR(S): Nakamura, Akio; Koshinuma, Masakatsu; Tajima, Kazuo  
 CORPORATE SOURCE: Nagoya Munic. Women's Coll., Nagoya, 464, Japan  
 SOURCE: Colloids and Surfaces (1992), 67, 183-93  
 CODEN: COSUD3; ISSN: 0166-6622  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 IT 27373-56-4, N-Decyl- $\beta$ -alanine 27373-57-5  
 41331-11-7 77390-89-7, N-Butyl- $\beta$ -alanine  
 RL: PRP (Properties)  
 (micelles, copper(II) complex solubilization in)  
 RN 27373-56-4 HCAPLUS  
 CN  $\beta$ -Alanine, N-decyl- (8CI, 9CI) (CA INDEX NAME)

$\text{Me}-(\text{CH}_2)_9-\text{NH}-\text{CH}_2-\text{CH}_2-\text{CO}_2\text{H}$

RN 27373-57-5 HCAPLUS  
 CN  $\beta$ -Alanine, N-octyl- (6CI, 8CI, 9CI) (CA INDEX NAME)

$\text{Me}-(\text{CH}_2)_7-\text{NH}-\text{CH}_2-\text{CH}_2-\text{CO}_2\text{H}$

RN 41331-11-7 HCAPLUS  
 CN  $\beta$ -Alanine, N-hexyl- (9CI) (CA INDEX NAME)

$\text{Me}-(\text{CH}_2)_5-\text{NH}-\text{CH}_2-\text{CH}_2-\text{CO}_2\text{H}$

RN 77390-89-7 HCAPLUS  
 CN  $\beta$ -Alanine, N-butyl- (9CI) (CA INDEX NAME)

$n\text{-BuNH}-\text{CH}_2-\text{CH}_2-\text{CO}_2\text{H}$

IT 27373-56-4D, N-Decyl- $\beta$ -alanine, copper(II) complexes  
 27373-57-5D, copper(II) complexes 41331-11-7D,  
 copper(II) complexes 77390-89-7D, N-Butyl- $\beta$ -alanine,  
 copper(II) complexes  
 RL: PROC (Process)  
 (solubilization of, in alkyl- $\beta$ -alanine micellar solns.)  
 RN 27373-56-4 HCAPLUS  
 CN  $\beta$ -Alanine, N-decyl- (8CI, 9CI) (CA INDEX NAME)

$\text{Me}-(\text{CH}_2)_9-\text{NH}-\text{CH}_2-\text{CH}_2-\text{CO}_2\text{H}$

RN 27373-57-5 HCAPLUS  
 CN  $\beta$ -Alanine, N-octyl- (6CI, 8CI, 9CI) (CA INDEX NAME)

$\text{Me}-(\text{CH}_2)_7-\text{NH}-\text{CH}_2-\text{CH}_2-\text{CO}_2\text{H}$

RN 41331-11-7 HCAPLUS  
 CN  $\beta$ -Alanine, N-hexyl- (9CI) (CA INDEX NAME)

Me- (CH<sub>2</sub>)<sub>5</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-CO<sub>2</sub>H

RN 77390-89-7 HCAPLUS  
CN β-Alanine, N-butyl- (9CI) (CA INDEX NAME)

n-BuNH-CH<sub>2</sub>-CH<sub>2</sub>-CO<sub>2</sub>H

AB The solubilization of the Cu(II) N-alkyl-β-alanine complexes (NAA; alkyl = Bu, NBuA; hexyl, NHeA; octyl, NOA; decyl, NDeA) in NAA aqueous micellar solns. was studied. A crystalline coordination compound of Cu:NAA composition 1:2 (the complex trans-[Cu(NAA)<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub>]) is formed by direct mixing of NAA with CuCl<sub>2</sub> aqueous solns. The amount of the insol. stoichiometric 1:2 complex increases with increasing NAA concentration below the NAA critical micelle

concentration (CMC), but the 1:2 complex begins to redissolve above the CMC and disappears at a certain NAA concentration (i.e.. the insol. 1:2 complex is solubilized in the NAA micelles). Visible spectroscopic data suggest that the dielec. environment around the Cu(II) ion coordination sphere in the solubilized 1:2 complex is similar to that in the crystalline 1:2 complex mol. Lamellar structures of NAA micelles solubilizing the 1:2 complexes were characterized by small-angle x-ray diffractometry. A model for the solubilization is proposed: 2 hydrocarbon chains in a 1:2 complex mol. of trans form are interlinked with the NAA bilayers. The free energy of solubilization was estimated from the solubilized amts. of the 1:2 complexes for the NDeA and NOA systems. The change in the free energy of solubilization per CH<sub>2</sub> group is -1.04 kJ mol<sup>-1</sup>, which is roughly half of the corresponding value for soap micellization.

L38 ANSWER 8 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1992:59021 HCAPLUS

DOCUMENT NUMBER: 116:59021

TITLE: Diethyl bromophosphate as a new condensing reagent for the formation of β-lactams from β-amino acids

AUTHOR(S): Chung, Bong Young; Paik, Kyu Cheol; Nah, Cha Soo  
CORPORATE SOURCE: Dep. Chem., Korea Univ., Seoul, 136-701, S. Korea  
SOURCE: Bulletin of the Korean Chemical Society (1991), 12(5), 589

CODEN: BKCSDE; ISSN: 0253-2964

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 116:59021

IT 16217-35-9

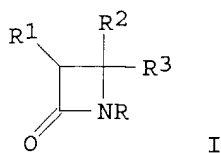
RL: RCT (Reactant); RACT (Reactant or reagent)  
(lactamization of, by bromophosphate)

RN 16217-35-9 HCAPLUS

CN β-Alanine, N-(1-methylethyl)- (9CI) (CA INDEX NAME)

i-PrNH-CH<sub>2</sub>-CH<sub>2</sub>-CO<sub>2</sub>H

GI



AB  $\beta$ -Lactams I ( $R = \text{CH}_2\text{Ph}$ ,  $\text{CHMe}_2$ ,  $\text{H}$ ;  $\text{R}_1$ ,  $\text{R}_3 = \text{H}$ ,  $\text{Me}$ ;  $\text{R}_2 = \text{H}$ ,  $\text{Me}$ ,  $\text{CO}_2\text{Me}$ ,  $\text{Ph}$ ) were obtained in 25-89% yield by cyclizing  $\text{HO}_2\text{CCHR}_1\text{CR}_2\text{R}_3\text{NHR}$  with  $\text{BrP}(\text{O})(\text{OEt})_2$ .

L38 ANSWER 9 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1991:631922 HCAPLUS

DOCUMENT NUMBER: 115:231922

TITLE: A convenient method for the  $\beta$ -lactam formation from  $\beta$ -amino acids using triphenylphosphine-hexachloroethane-triethylamine-acetonitrile system

AUTHOR(S): Chung, Bong Young; Paik, Kyu Cheol; Nah, Cha Soo  
CORPORATE SOURCE: Dep. Chem., Korea Univ., Seoul, 136-701, S. Korea  
SOURCE: Bulletin of the Korean Chemical Society (1991), 12(4), 456

CODEN: BKCSDE; ISSN: 0253-2964

DOCUMENT TYPE: Journal

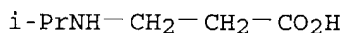
LANGUAGE: English

IT 16217-35-9

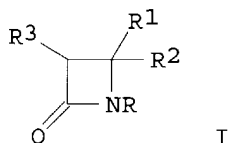
RL: RCT (Reactant); RACT (Reactant or reagent)  
(intramol. cyclocondensation of,  $\beta$ -lactam from)

RN 16217-35-9 HCAPLUS

CN  $\beta$ -Alanine, N-(1-methylethyl)- (9CI) (CA INDEX NAME)



GI



AB Intramol cyclocondensation of  $\text{RNHCR}_1\text{R}_2\text{CHR}_3\text{CO}_2\text{H}$  ( $R = \text{H}$ ,  $\text{CHMe}_2$ ,  $\text{CH}_2\text{Ph}$ ;  $\text{R}_1 = \text{H}$ ,  $\text{Me}$ ,  $\text{Ph}$ ,  $\text{CO}_2\text{Me}$ ;  $\text{R}_2$ ,  $\text{R}_3 = \text{H}$ ,  $\text{Me}$ ) in the presence of the title reagent/solvent system gave 70-92%  $\beta$ -lactams I.

L38 ANSWER 10 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1991:27105 HCAPLUS

DOCUMENT NUMBER: 114:27105

TITLE: Absorbent composition containing a severely-hindered amine mixture with amine salts and/or amino acid additives for the absorption of hydrogen sulfide

INVENTOR(S): Ho, W. S. Winston; Sartori, Guido; Stogryn, Eugene L.

PATENT ASSIGNEE(S): Exxon Research and Engineering Co., USA

SOURCE: U.S., 19 pp. Cont. of U.S. Ser. No. 106,782,

abandoned.  
CODEN: USXXAM  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4961873	A	19901009	US 1989-398346	19890824 <--
PRIORITY APPLN. INFO.:			US 1987-106782	19871013 <--
OTHER SOURCE(S):	MARPAT 114:27105			
IT 58482-93-2, N-tert-Butylglycine				
RL: USES (Uses)				
	(absorbents containing, two severely-hindered amines in, for selective removal of hydrogen sulfide from gases)			
RN 58482-93-2 HCAPLUS				
CN Glycine, N-(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)				

t-BuNH-CH<sub>2</sub>-CO<sub>2</sub>H

AB An alkaline absorbent solution that reduces the H<sub>2</sub>S content in a treated gas to <10 ppm contains 2 severely-hindered amines, e.g., bis(t-butylaminoethoxy)ethane and ethoxyethoxyethanol-tert-butylamine, a severely-hindered amine salt, and/or a severely-hindered amino acid. The process is also suitable for the selective removal of H<sub>2</sub>S from liquid mixts. comprising H<sub>2</sub>S and CO<sub>2</sub>.

L38 ANSWER 11 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 1990:201962 HCAPLUS  
DOCUMENT NUMBER: 112:201962  
TITLE: Addition of severely-hindered amine salts and/or amino acids to non-hindered amine solutions for the absorption of hydrogen sulfide  
INVENTOR(S): Ho, W. S. Winston; Sartori, Guido  
PATENT ASSIGNEE(S): Exxon Research and Engineering Co., USA  
SOURCE: U.S., 13 pp.  
CODEN: USXXAM  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4892674	A	19900109	US 1987-106805	19871013 <--
PRIORITY APPLN. INFO.:			US 1987-106805	19871013 <--
OTHER SOURCE(S):	MARPAT 112:201962			
IT 58482-93-2, N-tert-Butylglycine				
RL: USES (Uses)				
	(absorbents containing, and severely-hindered amine salts and non-hindered amines, for hydrogen sulfide removal from gases)			
RN 58482-93-2 HCAPLUS				
CN Glycine, N-(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)				

t-BuNH-CH<sub>2</sub>-CO<sub>2</sub>H

AB An alkaline absorbent solution for the selective removal of H<sub>2</sub>S from a H<sub>2</sub>S-containing gas contains the additive of a severely-hindered amine salt, e.g., ethoxyethanol-tert-butylamine, and/or a severely-hindered amino acid, e.g., N-tert-butylalanine, to a non-hindered amine such as N-methyldiethanolamine (I). The H<sub>2</sub>S-removal process is also suitable for the gas mixts. containing H<sub>2</sub>S and CO<sub>2</sub>. Use of the above absorbent solution leads to higher selectivity for H<sub>2</sub>S than observed when I is used alone.

L38 ANSWER 12 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1990:182789 HCAPLUS

DOCUMENT NUMBER: 112:182789

TITLE: Addition of severely hindered amino acids to severely hindered amines for absorption of hydrogen sulfide

INVENTOR(S): Sartori, Guido; Ho, W. S. Winston

PATENT ASSIGNEE(S): Exxon Research and Engineering Co., USA

SOURCE: U.S., 10 pp.  
CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4895670	A	19900123	US 1987-106795	19871013 <--
PRIORITY APPLN. INFO.:			US 1987-106795	19871013 <--

OTHER SOURCE(S): CASREACT 112:182789

IT 58482-93-2, N-tert-Butylglycine

RL: **USES (Uses)**

(absorbents containing severely hindered amines and, for absorption of hydrogen sulfide)

RN 58482-93-2 HCAPLUS

CN Glycine, N-(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)

t-BuNH-CH<sub>2</sub>-CO<sub>2</sub>H

AB A process for the removal of H<sub>2</sub>S from fluid mixts. comprises using an alkaline absorbent solution containing a severely hindered amino acid and a severely hindered amine each having a cumulative -Es value (Taft's steric hindrance constant) >1.75. The process is also suitable for the selective removal of H<sub>2</sub>S from fluid mixts. containing H<sub>2</sub>S and CO<sub>2</sub>. Use of the absorbent solution leads to higher selectivity for H<sub>2</sub>S than observed when the severely hindered amine is used alone without the severely hindered amino acid. Suitable amino acid includes N-tert-butylalanine, N-tert-butylglycine, and their mixture

L38 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1989:38631 HCAPLUS

DOCUMENT NUMBER: 110:38631

TITLE: Preparation and use of acylaminopropionates as surfactants, emulsifiers, wetters, detergent components, and in production of waterproof leather

INVENTOR(S): Dahmen, Kurt; Mertens, Richard; Stockhausen, Dolf

PATENT ASSIGNEE(S): Chemische Fabrik Stockhausen G.m.b.H., Fed. Rep. Ger.

SOURCE: Ger. Offen., 9 pp.

CODEN: GWXXBX  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 FAMILY ACC. NUM. COUNT: 2  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3717961	A1	19880505	DE 1987-3717961	19870527 <--
DE 3717961	C2	19940526		
EP 265818	A2	19880504	EP 1987-115365	19871021 <--
EP 265818	A3	19900425		
EP 265818	B1	19940928		
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, NL, SE				
JP 63112544	A2	19880517	JP 1987-266178	19871021 <--
JP 2577011	B2	19970129		
ES 2003836	T3	19941216	ES 1987-115365	19871021 <--
AU 8780101	A1	19880428	AU 1987-80101	19871023 <--
AU 602171	B2	19901004		
BR 8705693	A	19880531	BR 1987-5693	19871023 <--
SU 1833368	A3	19930807	SU 1989-4613176	19890104 <--
RU 2062302	C1	19960620	RU 1989-4613251	19890104 <--
LV 11044	B	19961020	LV 1993-715	19930628 <--
LT 3617	B	19951227	LT 1993-1535	19931206 <--
LT 3805	B	19960325	LT 1993-1597	19931215 <--
PRIORITY APPLN. INFO.:			DE 1986-3636497	19861027 <--
			DE 1987-3717961	19870527 <--

OTHER SOURCE(S): MARPAT 110:38631

IT 112-87-8P 10488-59-2P 41331-11-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (preparation and acylation of, by maleic anhydride)

RN 112-87-8 HCAPLUS

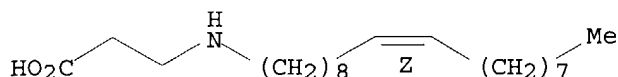
CN  $\beta$ -Alanine, N-octadecyl- (6CI, 8CI, 9CI) (CA INDEX NAME)

Me- (CH<sub>2</sub>)<sub>17</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-CO<sub>2</sub>H

RN 10488-59-2 HCAPLUS

CN  $\beta$ -Alanine, N-(9Z)-9-octadecenyl- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 41331-11-7 HCAPLUS

CN  $\beta$ -Alanine, N-hexyl- (9CI) (CA INDEX NAME)

Me- (CH<sub>2</sub>)<sub>5</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-CO<sub>2</sub>H

AB R1(R2A)NCH2CHR3CO2X [R1 = C1-22 (unsatd.) alkyl, alkoxyalkyl; R2 = C1-18 alkyl, C3-4 carboxyalkyl, carboxyphenyl, carboxy; R3 = H, Me; X = H, alkali metal, alkaline earth metal, (alkyl)ammonium alkanolammonium; A = CO, SO<sub>2</sub>, CONH, C0-3 alkylene] useful as emulsifiers, wetteners, surfactants,

and in preparation of waterproofing agents for leather, were prepared by reaction of R<sub>1</sub>NH<sub>2</sub> with (meth)acrylic acid followed by acylation with carboxylic acid anhydrides, carbonyl chlorides, isocyanates, etc. Thus, CH<sub>2</sub>:CHCO<sub>2</sub>H was added to oleylamine at 60° and after 2.5 h and 90° maleic anhydride was added and the mixture was stirred for a further 2 h at 70-80° to give N-oleyl-N-(2-carboxyethyl)maleamic acid. The latter was used to prepare waterproof leather.

L38 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1987:440328 HCAPLUS  
 DOCUMENT NUMBER: 107:40328  
 TITLE: Amine dealkylation  
 INVENTOR(S): Miller, William Harold; Balthazor, Terry Mack  
 PATENT ASSIGNEE(S): Monsanto Co., USA  
 SOURCE: Eur. Pat. Appl., 14 pp.  
 CODEN: EPXXDW  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 199702	A1	19861029	EP 1986-870047	19860421 <--
EP 199702	B1	19881221		
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
US 4804500	A	19890214	US 1986-841149	19860319 <--
DK 8601811	A	19861023	DK 1986-1811	19860421 <--
AU 8656410	A1	19861030	AU 1986-56410	19860421 <--
AU 580153	B2	19890105		
JP 61249955	A2	19861107	JP 1986-91967	19860421 <--
JP 06062522	B4	19940817		
ZA 8602986	A	19870225	ZA 1986-2986	19860421 <--
HU 43998	A2	19880128	HU 1986-1665	19860421 <--
HU 199399	B	19900228		
AT 39349	E	19890115	AT 1986-870047	19860421 <--
CA 1269665	A1	19900529	CA 1986-507122	19860421 <--
IL 78551	A1	19901223	IL 1986-78551	19860421 <--
PRIORITY APPLN. INFO.:			US 1985-725856	19850422 <--
			EP 1986-870047	19860421 <--
IT 3183-21-9 108957-96-6				
RL: RCT (Reactant); RACT (Reactant or reagent)				
(N-deisopropylation of)				
RN 3183-21-9 HCAPLUS				
CN Glycine, N-(1-methylethyl)- (9CI) (CA INDEX NAME)				

i-PrNH-CH<sub>2</sub>-CO<sub>2</sub>H

RN 108957-96-6 HCAPLUS  
 CN Glycine, N-methyl-N-(1-methylethyl)- (9CI) (CA INDEX NAME)

Me  
 |  
 i-Pr-N-CH<sub>2</sub>-CO<sub>2</sub>H

AB Substituted amines  $R_1NR_2R_3$  [ $R_1$  = acidic group containing at least one OH;  $R_2$  = H, Me,  $PhCH_2$ ,  $R_1$ ,  $R_3$ ;  $R_3$  =  $CR_4R_5CHR_6R_7$ ;  $R_2R_3N$  = heterocyclyl;  $R_4$ ,  $R_5$  = H, C1-6 alkyl, (un)substituted aryl;  $R_6$ ,  $R_7$  =  $R_4$ ,  $R_5$ , OH, C1-6 alkoxy, aryloxy, halo, SH, thioalkyl, mono- or dialkylamino, or, when  $R_6$  = H,  $R_7$  can be  $N(CH_2CO_2H)_2$ ] were dealkylated by heating at 250-400° in aqueous alkali, using at least the stoichiometric amount of alkali needed to neutralize the acidic OH groups, to give  $R_1R_2NH$  with removal of  $R_3$  groups as alkenes. The process is useful for preparation of valuable amino acids, e.g., glycine, sarcosine, iminodiacetic acid, and aminomethylphosphonic acid. Thus, a solution of 0.038 mol  $Me_2CHNMeCH_2CO_2H$  in  $H_2O$  containing 0.076

mol

NaOH was heated at 300° in an Monel autoclave to give 71% sarcosine.

L38 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN  
 ACCESSION NUMBER: 1986:462332 HCAPLUS  
 DOCUMENT NUMBER: 105:62332  
 TITLE: Surface treatment of zinc base materials  
 INVENTOR(S): Kurihara, Masao; Kimata, Shizuro; Imura, Hideaki; Naruse, Naohiko  
 PATENT ASSIGNEE(S): Toa Gosei Chemical Industry Co., Ltd., Japan  
 SOURCE: Jpn. Tokkyo Koho, 9 pp.  
 CODEN: JAXXAD  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 60056225	B4	19851209	JP 1978-102938	19780825 <--
JP 55031417	A2	19800305		

PRIORITY APPLN. INFO.: JP 1978-102938 19780825 <--  
 IT 41331-11-7 41421-76-5  
 RL: USES (Uses)  
 (pretreatment by aqueous alkalies and, of zinc, for coating with powdered epoxy resin)  
 RN 41331-11-7 HCAPLUS  
 CN  $\beta$ -Alanine, N-hexyl- (9CI) (CA INDEX NAME)

$Me-(CH_2)_5-NH-CH_2-CH_2-CO_2H$

RN 41421-76-5 HCAPLUS  
 CN Butanoic acid, 4-(dodecylamino)- (9CI) (CA INDEX NAME)

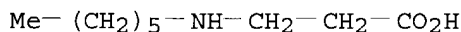
$Me-(CH_2)_{11}-NH-(CH_2)_3-CO_2H$

AB Surfaces of zinc are treated with aqueous alkali hydroxide and aqueous solns.  
 of  $RNHCnH_2nCO_2H$  ( $R$  = >C6 saturated or unsatd. aliphatic hydrocarbly groups,  $n > 2$ ) or H halide solns. and coated. Thus, Zn-plated steel was degreased, treated with 6% aqueous KOH, immersed 5 min at 90° in 3% aqueous hexyl- $\beta$ -aminopropionic acid, dried, electrostatically coated with a powdered epoxy resin, and baked to form a coating.

L38 ANSWER 16 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN



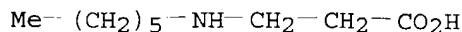
ACCESSION NUMBER: 1986:73067 HCAPLUS  
DOCUMENT NUMBER: 104:73067  
TITLE: Effect of surfactants on the formation of a metallic film during metalizing of glass fibers  
AUTHOR(S): Ermakov, E. A.; Pantaev, V. A.  
CORPORATE SOURCE: Kalinin. Gos. Univ., Kalinin, USSR  
SOURCE: Khim. Poverkhn.-Akt. Veshchestv Kompleksonov (1984), 107-10. Editor(s): Gorelov, I. P.  
Kalinin. Gos. Univ.: Kalinin, USSR.  
CODEN: 54JOAA  
DOCUMENT TYPE: Conference  
LANGUAGE: Russian  
IT 41331-11-7  
RL: USES (Uses)  
(surfactant, in electroless copper coating of glass fibers, film d. and structure in relation to)  
RN 41331-11-7 HCAPLUS  
CN  $\beta$ -Alanine, N-hexyl- (9CI) (CA INDEX NAME)



AB The effect of surfactants, i.e. Na alkylsulfates and alkyl- $\beta$ -alanine on the formation of a metal film during electroless Cu coating of glass fibers was studied. Elec. resistance of the fibers metalized without surfactants was substantially higher than that of samples prepared using the surfactants, which was associated with the difference in the Cu film surface defectiveness. Coatings obtained using the surfactants were distinguished by the fine-crystalline structure, whereas without them, coarser crystallites formed, and the coating was less dense. The best results in preparing dense coatings with fine-grained structure were observed when electroless bath contained Na undecylsulfate [1072-24-8] and N-hexyl- $\beta$ -alanine [41331-11-7].

L38 ANSWER 17 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1986:24719 HCAPLUS  
DOCUMENT NUMBER: 104:24719  
TITLE: Effect of inorganic salts of tin and palladium on colloidal-chemical properties of surfactants  
AUTHOR(S): Voronchikhina, L. I.; Pavlova, L. A.  
CORPORATE SOURCE: Kalinin. Gos. Univ., Kalinin, USSR  
SOURCE: Khim. Poverkhn.-Akt. Veshchestv Kompleksonov (1984), 88-92. Editor(s): Gorelov, I. P.  
Kalinin. Gos. Univ.: Kalinin, USSR.  
CODEN: 54JOAA  
DOCUMENT TYPE: Conference  
LANGUAGE: Russian  
IT 41331-11-7  
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)  
(surface activity of, in presence of tin or palladium chlorides)  
RN 41331-11-7 HCAPLUS  
CN  $\beta$ -Alanine, N-hexyl- (9CI) (CA INDEX NAME)



AB The behavior of colloidal solns. of surfactants (amphoteric

N-dodecyl-N,N-dimethyl- $\alpha$ -betain and N-ketyl- $\beta$ -alanine; anionic Na cetyl sulfate and Na undecyl sulfate and cationic decylpyridinium chloride and dodecylbenzyltrimethylammonium chloride) was studied in the presence of SnCl<sub>2</sub> and PdCl<sub>2</sub>. The saturated adlayer formation, critical micellization concentration, and surface tension were determined At < 0.5M SnCl<sub>2</sub> and PdCl<sub>2</sub> in solns., surface activity of the amphoteric and anionic surfactants increases significantly. The cationic surfactants are unstable in the presence of > 0.05M surfactants.

L38 ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1980:147180 HCAPLUS  
DOCUMENT NUMBER: 92:147180  
TITLE: Cation-binding cyclic peptides with lipophilic tails  
AUTHOR(S): Deber, C. M.; Adawadkar, P. D.  
CORPORATE SOURCE: Res. Inst., Hosp. Sick Child., Toronto, ON, M5G 1X8, Can.  
SOURCE: Biopolymers (1979), 18(10), 2375-96  
CODEN: BIPMAA; ISSN: 0006-3525  
DOCUMENT TYPE: Journal  
LANGUAGE: English

IT 20933-56-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and esterification of, with benzyl alc.)

RN 20933-56-6 HCAPLUS

CN Glycine, N-decyl- (8CI, 9CI) (CA INDEX NAME)

Me- (CH<sub>2</sub>)<sub>9</sub>-NH-CH<sub>2</sub>-CO<sub>2</sub>H

IT 41331-10-6P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 41331-10-6 HCAPLUS

CN Glycine, N-hexyl- (9CI) (CA INDEX NAME)

Me- (CH<sub>2</sub>)<sub>5</sub>-NH-CH<sub>2</sub>-CO<sub>2</sub>H

AB Cyclo[Glu(OCH<sub>2</sub>Ph)-Sar-Gly-NRCH<sub>2</sub>CO]<sub>2</sub> (I; Sar = NMeCH<sub>2</sub>CO, R = Me) was prepared by coupling BOC-Glu(OCH<sub>2</sub>Ph)-Sar-Gly-Sar-OH (BOC = Me<sub>3</sub>CO<sub>2</sub>C) to H-Glu(OCH<sub>2</sub>Ph)-Sar-Gly-Sar-OH by the mixed anhydride method, esterifying the resulting octapeptide with HOC<sub>6</sub>H<sub>4</sub>NO<sub>2</sub>-p, BOC-deblocking the resulting p-nitrophenyl ester with HCl, and cyclizing the resulting H-[Glu(OCH<sub>2</sub>Ph)-Sar-Gly-Sar]<sub>2</sub>-OC<sub>6</sub>H<sub>4</sub>NO<sub>2</sub>-p in DMF/pyridine at high dilution I [R = decyl (II), hexyl, cyclohexyl], cyclo[Glu(OCH<sub>2</sub>Ph)-Sar-Gly-Sar-Glu(OCH<sub>2</sub>Ph)-Sar-Gly-NR<sub>1</sub>CH<sub>2</sub>CO]<sub>2</sub> (R<sub>1</sub> = decyl), and cyclo(Phe-Sar-Gly-Sar)<sub>2</sub> were also prepared, and the above  $\alpha$ -benzyl esters were converted to the free acids. Proton and <sup>13</sup>C NMR data showed that I with a mixture of cis/trans peptide bond conformers were converted to the C<sub>2</sub>-sym. all-trans conformers upon complexation with Ca<sup>2+</sup>. II mediated the transport of cations across a thick-liquid membrane with the following selectivity: Ca<sup>2+</sup> > Na<sup>+</sup> > K<sup>+</sup> > Mn<sup>2+</sup> > Cu<sup>2+</sup> > Mg<sup>2+</sup> > Co<sup>2+</sup> > Zn<sup>2+</sup>.

L38 ANSWER 19 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1977:135270 HCAPLUS

DOCUMENT NUMBER: 86:135270

TITLE: Facilitated diffusion of amino acids across  
bimolecular lipid membranes as a model for selective  
accumulation of amino acids in a primordial protocell

AUTHOR(S): Stillwell, William

CORPORATE SOURCE: Dep. Biophys., Michigan State Univ., East Lansing, MI,  
USA

SOURCE: BioSystems (1976), 8(3), 111-17  
CODEN: BSYMBO; ISSN: 0303-2647

DOCUMENT TYPE: Journal

LANGUAGE: English

IT 627-01-0 3182-81-8 41331-10-6  
50997-13-2

RL: PEP (Physical, engineering or chemical process); PROC (Process)  
(diffusion of, across lipid membrane)

RN 627-01-0 HCAPLUS

CN Glycine, N-ethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

EtNH-CH<sub>2</sub>-CO<sub>2</sub>H

RN 3182-81-8 HCAPLUS

CN Glycine, N-butyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

n-BuNH-CH<sub>2</sub>-CO<sub>2</sub>H

RN 41331-10-6 HCAPLUS

CN Glycine, N-hexyl- (9CI) (CA INDEX NAME)

Me-(CH<sub>2</sub>)<sub>5</sub>-NH-CH<sub>2</sub>-CO<sub>2</sub>H

RN 50997-13-2 HCAPLUS

CN Glycine, N-nonyl- (9CI) (CA INDEX NAME)

Me-(CH<sub>2</sub>)<sub>8</sub>-NH-CH<sub>2</sub>-CO<sub>2</sub>H

AB A simple transport system for the uptake of amino acids into lipid vesicles was studied as a model for the protocell. The rate of diffusion of amino acids across bimol. lipid membranes was greatly stimulated by water-soluble aldehydes. Even HCHO was an effective carrier, although pyridoxal was much more effective. Series of reduced amino acid imines of glycine, lysine, and histidine were synthesized to measure the relative abilities of different aldehydes as carriers for amino acids. Comparison of partition coeffs. to the diffusion rates of the derivatized amino acids indicated that the more lipophilic derivs. are more readily diffused. This simple type of facilitated diffusion makes lipid vesicles an attractive model of the 1st primordial cell.

L38 ANSWER 20 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1976:430029 HCAPLUS

DOCUMENT NUMBER: 85:30029

TITLE: Oxidation of sarcosine and N-alkyl derivatives of  
glycine by D-amino-acid oxidase

AUTHOR(S): Naoi, Makoto; Yagi, Kunio

CORPORATE SOURCE: Fac. Med., Univ. Nagoya, Nagoya, Japan  
SOURCE: Biochimica et Biophysica Acta (1976),  
438(1), 61-70  
CODEN: BBACAQ; ISSN: 0006-3002  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
IT 627-01-0 3182-81-8 25303-14-4  
35386-27-7 41331-10-6  
RL: BIOL (Biological study)  
(amino acid oxidase specificity for)  
RN 627-01-0 HCAPLUS  
CN Glycine, N-ethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

EtNH-CH<sub>2</sub>-CO<sub>2</sub>H

RN 3182-81-8 HCAPLUS  
CN Glycine, N-butyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

n-BuNH-CH<sub>2</sub>-CO<sub>2</sub>H

RN 25303-14-4 HCAPLUS  
CN Glycine, N-propyl- (6CI, 8CI, 9CI) (CA INDEX NAME)

n-PrNH-CH<sub>2</sub>-CO<sub>2</sub>H

RN 35386-27-7 HCAPLUS  
CN Glycine, N-pentyl- (6CI, 9CI) (CA INDEX NAME)

Me-(CH<sub>2</sub>)<sub>4</sub>-NH-CH<sub>2</sub>-CO<sub>2</sub>H

RN 41331-10-6 HCAPLUS  
CN Glycine, N-hexyl- (9CI) (CA INDEX NAME)

Me-(CH<sub>2</sub>)<sub>5</sub>-NH-CH<sub>2</sub>-CO<sub>2</sub>H

AB Sarcosine was oxidized by D-amino acid oxidase (EC 1.4.3.3) to yield methylamine and glyoxylic acid. A series of N-alkyl glycines were also oxidized by this enzyme. N-acetyl- and N-phenylglycine inhibited the oxidase by competing with the substrate, whereas N-methyl-N-acetyl glycine did not bind to the enzyme. This suggests the requirement of at least 1 unsubstituted H atom at the amino group of glycine for binding. The primary step in the reaction was the release of a proton from the substrate, indicating the formation of a substituted imino acid, which was spontaneously hydrolyzed to glyoxylic acid and an amine.

L38 ANSWER 21 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 1975:514857 HCAPLUS  
DOCUMENT NUMBER: 83:114857  
TITLE: Preparation of N-alkyl and N-arylglycines from glyoxylic acid using carbonylhydridoferrate as a

reducing agent  
AUTHOR(S): Watanabe, Yoshihisa; Shim, Sang Chul; Mitsudo,  
Takeaki; Yamashita, Masakazu; Takegami, Yoshinobu  
CORPORATE SOURCE: Fac. Eng., Kyoto Univ., Kyoto, Japan  
SOURCE: Chemistry Letters (1975), (7), 699-700  
CODEN: CMLTAG; ISSN: 0366-7022  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
IT 3182-82-9P 56676-69-8P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)  
RN 3182-82-9 HCAPLUS  
CN Glycine, N-butyl-, hydrochloride (7CI, 8CI, 9CI) (CA INDEX NAME)

n-BuNH-CH<sub>2</sub>-CO<sub>2</sub>H

● HCl

RN 56676-69-8 HCAPLUS  
CN Glycine, N-hexyl-, hydrochloride (9CI) (CA INDEX NAME)

Me-(CH<sub>2</sub>)<sub>5</sub>-NH-CH<sub>2</sub>-CO<sub>2</sub>H

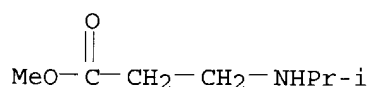
● HCl

AB To Fe(CO)<sub>5</sub> and alc. in KOH was added an amine, glyoxylic acid and EtOH and  
the mixture stirred 24 hr at room temperature The precipitate was acidified  
with concentrate  
HCl to give salts of glycines, RNHCH<sub>2</sub>CO<sub>2</sub>H·HCl (R = Me, Bu, hexyl,  
cyclohexyl, PhCH<sub>2</sub>, Ph, p-MeC<sub>6</sub>H<sub>4</sub>, p-MeOC<sub>6</sub>H<sub>4</sub>, p-ClC<sub>6</sub>H<sub>4</sub>, β-naphthyl.

L38 ANSWER 22 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 1975:409540 HCAPLUS  
DOCUMENT NUMBER: 83:9540  
TITLE: Alkyl 5-oxoalkanoates  
INVENTOR(S): Mueller, Werner  
PATENT ASSIGNEE(S): Farbwerke Hoechst A.-G.  
SOURCE: Ger. Offen., 11 pp.  
CODEN: GWXXBX  
DOCUMENT TYPE: Patent  
LANGUAGE: German  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

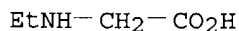
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2325160	A1	19741205	DE 1973-2325160	19730518 <--
ZA 7402951	A	19750528	ZA 1974-2951	19740508 <--
IN 141915	A	19770430	IN 1974-CA1033	19740509 <--
NL 7406400	A	19741120	NL 1974-6400	19740513 <--
CH 593902	A	19771230	CH 1974-6689	19740515 <--
IT 1012464	A	19770310	IT 1974-22850	19740516 <--

FR 2229679 A1 19741213 FR 1974-17272 19740517 <--  
 FR 2229679 B1 19781117  
 JP 50030829 A2 19750327 JP 1974-54612 19740517 <--  
 BE 815282 A1 19741120 BE 1974-144528 19740520 <--  
 GB 1473184 A 19770511 GB 1974-22412 19740520 <--  
 PRIORITY APPLN. INFO.: DE 1973-2325160 19730518 <--  
 IT 42313-51-9  
 RL: CAT (Catalyst use); **USES (Uses)**  
 (catalyst, for ketone addition to alkyl acrylates)  
 RN 42313-51-9 HCAPLUS  
 CN  $\beta$ -Alanine, N-(1-methylethyl)-, methyl ester (9CI) (CA INDEX NAME)

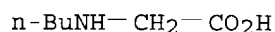


AB Fifteen RCOCHR1CH2CHR2CO2R3 [R = Me, Et, Bu, or Ph; R1 = H, Me, Pr, or Ph; or RR1 = (CH2)4; R2 = H or Me; R3 = C1-4 alkyl] or their mixts. were prepared by reaction of RCOCH2R1 with CH2:CR2CO2R3 in the presence of amines. Thus, Me2CO and CH2:CHCO2Me were autoclaved in the presence of aqueous Me2CHNH2 and BzOH at 180° to give 84.5% MeCO(CH2)3CO2Me and < 10% (MeO2CCH2CH2)2CHCOMe.

L38 ANSWER 23 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN  
 ACCESSION NUMBER: 1974:888 HCAPLUS  
 DOCUMENT NUMBER: 80:888  
 TITLE: Diffusion of glycine and N-substituted glycines across bimolecular lipid membranes  
 AUTHOR(S): Stillwell, William; Winter, Harry C.  
 CORPORATE SOURCE: Dep. Biochem., Pennsylvania State Univ., University Park, PA, USA  
 SOURCE: Biochemical and Biophysical Research Communications (1973), 54(4), 1437-43  
 CODEN: BBRCA9; ISSN: 0006-291X  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 IT 627-01-0 3182-81-8 41331-10-6 50997-13-2  
 RL: PEP (Physical, engineering or chemical process); PROC (Process) (diffusion of, across liposome)  
 RN 627-01-0 HCAPLUS  
 CN Glycine, N-ethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RN 3182-81-8 HCAPLUS  
 CN Glycine, N-butyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RN 41331-10-6 HCAPLUS  
 CN Glycine, N-hexyl- (9CI) (CA INDEX NAME)

Me- (CH<sub>2</sub>)<sub>5</sub>-NH-CH<sub>2</sub>-CO<sub>2</sub>H

RN 50997-13-2 HCAPLUS  
CN Glycine, N-nonyl- (9CI) (CA INDEX NAME)

Me- (CH<sub>2</sub>)<sub>8</sub>-NH-CH<sub>2</sub>-CO<sub>2</sub>H

AB Free glycine diffused very slowly across synthetic bimol. lipid membranes, whereas several N-substituted derivs. of glycine penetrated the membranes more readily. Pyridoxal, formaldehyde, and acetaldehyde enhanced the diffusion of glycine across the membranes, presumably the result of imine formation between the aldehyde and the  $\alpha$ -amino group of glycine. Several N-substituted glycines were synthesized and their rates of efflux from liposomes were related to their H<sub>2</sub>O-CHCl<sub>3</sub> partition coeffs. This is the 1st demonstration of carrier-mediated diffusion of amino acids across a bimol. lipid membrane.

L38 ANSWER 24 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1973:101277 HCAPLUS  
DOCUMENT NUMBER: 78:101277  
TITLE: Synergistic combinations for inhibiting the attack of  
alkaline solutions on alkali-sensitive substrates  
INVENTOR(S): Dupre, Jean; Booman, Keith A.  
PATENT ASSIGNEE(S): Rohm and Haas Co.  
SOURCE: U.S., 7 pp.  
CODEN: USXXAM  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 2  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3653095	A	19720404	US 1969-835906	19690618 <--
GB 1320793	A	19730620	GB 1970-29430	19700617 <--
PRIORITY APPLN. INFO.:			US 1969-834499	19690618 <--
			US 1969-835906	19690618 <--

IT 1462-54-0 41331-10-6 41331-11-7

RL: USES (Uses)  
(corrosion inhibition by, of alkaline solns.)

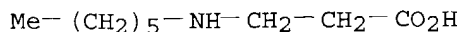
RN 1462-54-0 HCAPLUS  
CN  $\beta$ -Alanine, N-dodecyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

Me- (CH<sub>2</sub>)<sub>11</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-CO<sub>2</sub>H

RN 41331-10-6 HCAPLUS  
CN Glycine, N-hexyl- (9CI) (CA INDEX NAME)

Me- (CH<sub>2</sub>)<sub>5</sub>-NH-CH<sub>2</sub>-CO<sub>2</sub>H

RN 41331-11-7 HCAPLUS  
CN  $\beta$ -Alanine, N-hexyl- (9CI) (CA INDEX NAME)



AB During cleaning with an aqueous alkaline solution containing 0.1-10 weight % alkali, materials (e.g. Al, Zn, Sn, Pb, their alloys, Si oxides and compds. containing Si oxides) which are sensitive to the alkaline attack are protected by a synergistic combination of:  $\geq 1$  metal ion (0.005M) such as  $\text{Ba}^{2+}$ ,  $\text{Ca}^{2+}$ , and  $\text{Sr}^{2+}$  with  $\geq 1$  surface-active agent (0.5 weight %) selected from alkyl glycosides having a formula  $\text{ROGmH}$ , where G is a glycosyl radical, R is C6-16 alkyl connected to C-1 of the glycosyl radical through the O, and m = 1-4; or ethylene oxide adducts of the alkyl glycosides containing  $\leq 2$  ethylene oxide units per glycosyl radical; or amino carboxylic acids having  $\text{C} \geq 10$  and metal salts of amino carboxylic acids (0.01-5 weight %). Optionally in certain and essentially in other applications, a H<sub>2</sub>O-soluble naphthalene derivative may be added to the synergistic combination.

L38 ANSWER 25 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1973:38037 HCAPLUS

DOCUMENT NUMBER: 78:38037

TITLE: Potential hypotensive compounds. Substituted 3-aminopropionates and 3-aminopropionohydroxamic acids  
 AUTHOR(S): Biggs, D. F.; Coutts, R. T.; Selley, M. L.; Towill, G. A.

CORPORATE SOURCE: Fac. Pharm. Pharm. Sci., Univ. Alberta, Edmonton, AB, Can.

SOURCE: Journal of Pharmaceutical Sciences (1972), 61(11), 1739-45

CODEN: JPMSAE; ISSN: 0022-3549

DOCUMENT TYPE: Journal

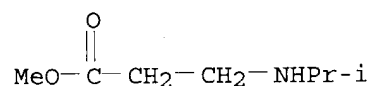
LANGUAGE: English

IT 40870-77-7P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation and hypotensive effect of)

RN 40870-77-7 HCAPLUS

CN  $\beta$ -Alanine, N-(1-methylethyl)-, methyl ester, hydrochloride (9CI) (CA INDEX NAME)



● HCl

AB Most of the 48 3-aminopropionate esters studied were synthesized by addition of an amine across the  $\alpha,\beta$ -double bond of Me acrylate [96-33-3], Me methacrylate [80-62-6], or Me crotonate [18707-60-3], while the remainder were obtained by interaction of 1 mole of a 3-bromopropionic ester with 2 moles of the corresponding amine. Twenty-six 3-aminopropionohydroxamic acid hydrochlorides were prepared by treatment of the appropriate amino ester with hydroxylamine-HCl [5470-11-1] in MeOH. Many of the compds. such as 2-methyl-3-[(2-phenylethyl)amino]propanoic acid Me ester [6297-67-2], 3,3'-[(2-phenylethyl)iminobis]propanoic acid dimethyl ester [38129-46-3], N-[3-(hydroxyamino)-2-methyl-3-



oxopropyl]heptanaminium chloride [38129-47-4], and N-[3-(hydroxyamino)-3-oxopropyl]-2-(2-phenylethyl)benzeneethanaminium chloride [38202-84-5] possessed hypotensive properties but of very short duration. 2-Methyl-3-(octylamino)propanoic acid Me ester [29228-46-4] was the most active, and at 4 mg/kg i.v. decreased the blood pressure of rats by an average of 52% for 12 min. Some of the compds. were screened for their ability to protect mice against a lethal dose of diisopropylfluorophosphate [55-91-4], but none was active.

L38 ANSWER 26 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1971:75986 HCAPLUS

DOCUMENT NUMBER: 74:75986

TITLE: Synthesis and properties of some hypotensive N-alkylaminopropionic esters and N,N-dialkylaminopropionic esters and their hydroxamic acids

AUTHOR(S): Coutts, Ronald T.; Hubbard, J. W.; Midha, Kamal K.; Prasad, Kailash

CORPORATE SOURCE: Fac. Pharm. Pharm. Sci., Univ. Alberta, Edmonton, AB, Can.

SOURCE: Journal of Pharmaceutical Sciences (1971), 60(1), 28-33

CODEN: JPMSAE; ISSN: 0022-3549

DOCUMENT TYPE: Journal

LANGUAGE: English

IT 10478-41-8P 31044-47-0P 31044-48-1P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

RN 10478-41-8 HCAPLUS

CN  $\beta$ -Alanine, N-ethyl- (7CI, 8CI, 9CI) (CA INDEX NAME)

$\text{EtNH}-\text{CH}_2-\text{CH}_2-\text{CO}_2\text{H}$

RN 31044-47-0 HCAPLUS

CN  $\beta$ -Alanine, N-hexyl-, methyl ester (8CI, 9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{O} \\ || \\ \text{MeO}-\text{C}-\text{CH}_2-\text{CH}_2-\text{NH}-(\text{CH}_2)_5-\text{Me} \end{array}$$

RN 31044-48-1 HCAPLUS

CN  $\beta$ -Alanine, N-hexyl-, methyl ester, hydrochloride (8CI, 9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{O} \\ || \\ \text{MeO}-\text{C}-\text{CH}_2-\text{CH}_2-\text{NH}-(\text{CH}_2)_5-\text{Me} \end{array}$$

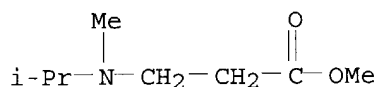
● HCl

GI For diagram(s), see printed CA Issue.

AB Thirty-eight 3-(N-alkylamino)- and 3-(N,N-dialkylamino)propionic esters

(I), hydroxamic acids (II), carboxylic acids, and related compds. were synthesized and the majority of the esters and hydroxamic acids decreased the blood pressure of anesthetized cats, while the carboxylic acids were inactive. The esters were prepared by the interaction of methyl acrylate or methyl methacrylate and an appropriate amine. Some hindered amines did not react with the acrylate, and some esters hydrolyzed to the corresponding carboxylic acids when stored even for a short time. The hydroxamic acids were prepared from the amino esters treated with hydroxylamine.

L38 ANSWER 27 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN  
 ACCESSION NUMBER: 1970:445265 HCAPLUS  
 DOCUMENT NUMBER: 73:45265  
 TITLE: Derivatives of substituted acetic acids. XXVIII.  
 Dialkylaminopropyl esters of  $\alpha$ -  
 naphthylheterylacetic acids  
 AUTHOR(S): Mndzhoyan, A. L.; Badalyan, V. E.  
 CORPORATE SOURCE: Inst. Tonkoi Org. Khim., Erevan, USSR  
 SOURCE: Armyanskii Khimicheskii Zhurnal (1970),  
 23(4), 258-67  
 CODEN: AYKZAN; ISSN: 0515-9628  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Russian  
 IT 27453-30-1P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 27453-30-1 HCAPLUS  
 CN  $\beta$ -Alanine, N-methyl-N-(1-methylethyl)-, methyl ester (9CI) (CA INDEX  
 NAME)



AB A mixture of 0.5 mole  $\text{R}_1\text{R}_2\text{NH}$ , 0.5 mole  $\text{CH}_2:\text{CHCO}_2\text{Me}$ , in 200 ml  $\text{C}_6\text{H}_6$  refluxed for 6-8 hr (with  $\text{iso-Pr}_2\text{NH}$ , the mixture was heated at  $95^\circ$  in a sealed tube 16-20 hr while with  $(\text{iso-Pr})_2\text{NH}$  similarly treated for 150 hr, to give  $\text{R}_1\text{R}_2\text{NCH}_2\text{CH}_2\text{CO}_2\text{Me}$  (I).  $\text{LiAlH}_4$  reduction of (I) gave  $\text{R}_1\text{R}_2\text{NCH}_2\text{CH}_2\text{CH}_2\text{OH}$  (II) which, in refluxing  $\text{PhMe}$ , reacted with  $\alpha\text{-C}_{10}\text{H}_7\text{CHClCOCl}$  (III) [from  $\alpha\text{-C}_{10}\text{H}_7\text{CH}(\text{OH})\text{CO}_2\text{H}$  (50.5 g) and refluxing  $\text{SOCl}_2$  (180 ml)] to give the corresponding  $\alpha\text{-C}_{10}\text{H}_7\text{CHClCO}_2(\text{CH}_2)_3\text{NR}_1\text{R}_2$  (IV). IV treated with an amine yielded the title  $\alpha\text{-C}_{10}\text{H}_7\text{CHR}_3\text{CO}_2(\text{CH}_2)_3\text{NR}_1\text{R}_2$  (V). Thus a mixture of 0.025 mole IV, 0.05 mole piperidine, and 100 ml  $\text{PhMe}$  refluxed 6-8 hr gave 77% V ( $\text{R}_1 = \text{R}_2 = \text{Me}$ ,  $\text{R}_3 = \text{piperidino}$ ), b<sub>3</sub> 228-30°. The morpholino analog was similarly prepared. Approx. 150 new compds. and derivs. were reported.

L38 ANSWER 28 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN  
 ACCESSION NUMBER: 1967:517255 HCAPLUS  
 DOCUMENT NUMBER: 67:117255  
 TITLE: Preparation of N-substituted aspartic esters,  
 $\beta$ -amino esters, and their corresponding acids  
 AUTHOR(S): Pfau, Michel  
 CORPORATE SOURCE: Lab. Chim. Ecole Norm. Super., Paris, Fr.  
 SOURCE: Bulletin de la Societe Chimique de France (  
 1967), (4), 1117-25  
 CODEN: BSCFAS; ISSN: 0037-8968  
 DOCUMENT TYPE: Journal

LANGUAGE: French  
OTHER SOURCE(S): CASREACT 67:117255  
IT 16217-35-9P 16270-07-8P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation and N.M.R. of)  
RN 16217-35-9 HCAPLUS  
CN  $\beta$ -Alanine, N-(1-methylethyl)- (9CI) (CA INDEX NAME)

i-PrNH-CH<sub>2</sub>-CH<sub>2</sub>-CO<sub>2</sub>H

RN 16270-07-8 HCAPLUS  
CN  $\beta$ -Alanine, N-propyl- (8CI, 9CI) (CA INDEX NAME)

n-PrNH-CH<sub>2</sub>-CH<sub>2</sub>-CO<sub>2</sub>H

AB Et acrylate (I), diethyl fumarate (II), dimethyl maleate (III), MeCH:CHCO<sub>2</sub>Et (IV), and CH<sub>2</sub>:CMeCO<sub>2</sub>Me (V) are treated with PrNH<sub>2</sub>, iso-PrNH<sub>2</sub>, and Et<sub>2</sub>NH to give amino acids. Thus, a mixture of 0.05 mole I and 0.5 mole PrNH<sub>2</sub> is kept 24 hrs. to give Et  $\beta$ -propylaminopropionate, b0.1 32°. A mixture of 5.0 g. I and 1.5 g. PrNH<sub>2</sub> is refluxed 10 hrs. to give diethyl  $\beta,\beta'$ -propyliminodipropionate, b0.4 98°. Also prepared are (reactants, product, b.p./mm., and m.p. given): iso-PrNH<sub>2</sub> and I, iso-PrNHCH<sub>2</sub>CH<sub>2</sub>CO<sub>2</sub>Et, 38°/0.4, -; iso-PrNH<sub>2</sub> and I, iso-PrN(CH<sub>2</sub>CH<sub>2</sub>CO<sub>2</sub>Et)<sub>2</sub>, 92°/0.05, -; Et<sub>2</sub>NH and I, Et<sub>2</sub>NCH<sub>2</sub>CH<sub>2</sub>CO<sub>2</sub>Et, 28°/0.08, -; PrNH<sub>2</sub> and IV, MeCH(NHPr)CH<sub>2</sub>CO<sub>2</sub>Et, 36°/0.15, -; iso-PrNH<sub>2</sub> and IV, Me(iso-PrNH)CHCH<sub>2</sub>CO<sub>2</sub>Et, 77°/11, -; PrNH<sub>2</sub> and V, PrNHCH<sub>2</sub>CHMeCO<sub>2</sub>Me, 31°/0.15, -; iso-PrNH<sub>2</sub> and V, iso-PrNHCH<sub>2</sub>CHMeCO<sub>2</sub>Me, 41°/0.1, -; PrNH<sub>2</sub> and III, MeO<sub>2</sub>CCH<sub>2</sub>CH(NHPr)CO<sub>2</sub>Me, 65-6°/0.15, -; iso-PrNH<sub>2</sub> and III, MeO<sub>2</sub>CCH<sub>2</sub>CH(NHPr-iso)CO<sub>2</sub>Me, 70°/0.3, -; Et<sub>2</sub>NH and III, MeO<sub>2</sub>CCH(NEt<sub>2</sub>)CH<sub>2</sub>CO<sub>2</sub>Me, 64°/0.3, -; PrNH<sub>2</sub> and II, EtO<sub>2</sub>CCH(NHPr)CH<sub>2</sub>CO<sub>2</sub>Et, 91°/0.3, -; iso-PrNH<sub>2</sub> and II, EtO<sub>2</sub>CCH(NHPr-iso)CH<sub>2</sub>CO<sub>2</sub>Et, 84°/0.4, -; Et<sub>2</sub>NH and II, EtO<sub>2</sub>CCH(NEt<sub>2</sub>)CH<sub>2</sub>CO<sub>2</sub>Et, 62°/0.1, -; piperidine and III, di-Me N,N-pentamethyleneaspartate, 98-101°/0.5, 44-4.5°; piperidine and III, Me  $\alpha$ -piperidino- $\beta$ -piperidinocarbonylpropionate, -, 182-3° (decomposition). Also prepared are iso-PrNHCHMeCH<sub>2</sub>CO<sub>2</sub>Et-HCl, m. 118.5-19.5°, and iso-PrNHCH<sub>2</sub>CHMeCO<sub>2</sub>Me.HCl, m. 114-14.5°. The esters are hydrolyzed to give the following acids (m.p. given): PrNHCH<sub>2</sub>CH<sub>2</sub>CO<sub>2</sub>H, 150.5-1.5°; iso-PrNHCH<sub>2</sub>CH<sub>2</sub>CO<sub>2</sub>H, 165-6°; Et<sub>2</sub>NCH<sub>2</sub>CH<sub>2</sub>CO<sub>2</sub>H, 68-70°; Me(PrNH)CHCH<sub>2</sub>CO<sub>2</sub>H, 142-3°; Me(iso-PrNH)CHCH<sub>2</sub>CO<sub>2</sub>H, 165-6°; PrNHCH<sub>2</sub>CHMeCO<sub>2</sub>H, 136-7°; iso-PrNHCH<sub>2</sub>CHMeCO<sub>2</sub>H, 170.5-1.0°; MeO<sub>2</sub>C(PrNH)CHCH<sub>2</sub>CO<sub>2</sub>H, 151°; MeO<sub>2</sub>C(iso-PrNH)CHCH<sub>2</sub>CO<sub>2</sub>H, 120.5-21°; EtO<sub>2</sub>C(PrNH)CHCH<sub>2</sub>CO<sub>2</sub>H, 165-7°; EtO<sub>2</sub>C(iso-PrNH)CHCH<sub>2</sub>CO<sub>2</sub>H, 94-5°, HO<sub>2</sub>CCH(NHPr-iso)CH<sub>2</sub>CO<sub>2</sub>H, 170-2°. N.M.R. data are given for the prepared compds.

L38 ANSWER 29 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 1966:451518 HCAPLUS  
DOCUMENT NUMBER: 65:51518  
ORIGINAL REFERENCE NO.: 65:9660g-h,9661a  
TITLE: Systemic fungicides  
INVENTOR(S): Harnack, Willy; Schwarz, Justus  
SOURCE: 3 pp.  
DOCUMENT TYPE: Patent

LANGUAGE: Unavailable

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	DD 45884		19660205	DD	19641224 <--
	GB 1048507			GB	
IT	542-53-0, Glycine, N-ethyl-, hydrochloride 627-01-0, Glycine, N-ethyl- 3182-82-9, Glycine, N-butyl-, hydrochloride 3182-86-3, Glycine, N-isobutyl-, hydrochloride 3183-23-1 , Glycine, N-isopropyl-, ethyl ester, hydrochloride 3338-22-5, Glycine, N-isopropyl-, hydrochloride 6939-13-5, Glycine, N-propyl-, hydrochloride (as fungicide)				
RN	542-53-0 HCAPLUS				
CN	Glycine, N-ethyl-, hydrochloride (7CI, 8CI, 9CI) (CA INDEX NAME)				

EtNH-CH<sub>2</sub>-CO<sub>2</sub>H

● HCl

RN 627-01-0 HCAPLUS  
CN Glycine, N-ethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

EtNH-CH<sub>2</sub>-CO<sub>2</sub>H

RN 3182-82-9 HCAPLUS  
CN Glycine, N-butyl-, hydrochloride (7CI, 8CI, 9CI) (CA INDEX NAME)

n-BuNH-CH<sub>2</sub>-CO<sub>2</sub>H

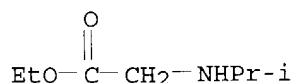
● HCl

RN 3182-86-3 HCAPLUS  
CN Glycine, N-(2-methylpropyl)-, hydrochloride (9CI) (CA INDEX NAME)

i-BuNH-CH<sub>2</sub>-CO<sub>2</sub>H

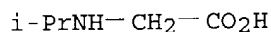
● HCl

RN 3183-23-1 HCAPLUS  
CN Glycine, N-(1-methylethyl)-, ethyl ester, hydrochloride (9CI) (CA INDEX NAME)



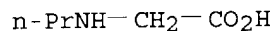
● HCl

RN 3338-22-5 HCAPLUS  
 CN Glycine, N-(1-methylethyl)-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 6939-13-5 HCAPLUS  
 CN Glycine, N-propyl-, hydrochloride (7CI, 8CI, 9CI) (CA INDEX NAME)



● HCl

AB Glycine derivs. of the general formula  $\text{RHNCH}_2\text{CO}_2\text{R}'$  ( $\text{R} = \text{H}, \text{Me}, \text{or Et}$ ) were systemic fungicides in vivo but not in vitro (spore germination test). Four young tomato plants with 4 or 5 leaves, in plastic pots were treated 2 times at 2-day intervals at the root stock with 3 ml. of test solution. Two days later they were sprayed with a spore suspension of *Phytophthora infestans*, then placed in a moist chamber. After 4 days each plant was scored for fungus infestation on scale 0, 1, 2, 3, or 4 meaning no, mild, median, marked infestation, or plant destroyed, resp. Scores for water alone and for each fungicide in replicate rests were summed. The sum for water was set at 100, and the relative scores of fungicides recorded. For 8 plants so treated with N-ethylglycine (I), N-ethylglycine-HCl (II), N-propylglycine-HCl (III), and N-2-hydroxyethylglycine (IV) in 0.5% solns., the relative infection scores were 0, 6, 10, 11, resp., and for 0.25% solns. 12, 10, 25, 20, resp. Eight plants sprayed sop. with solns. of II, III, and N-isopropylglycine-HCl were protected to a similar extent. Celery plants were protected against *Septoria apii* by root stock immersion in 0.5 and 0.25% solns. of the methyl esters and the methyl ester hydrochlorides of N-isopropylglycine and N-allylglycine, the Et ester of N-allylglycine, and N-butylglycine, N-isobutylglycine hydrochlorides. Areas of infection were usually smaller than in the controls. Development of reproductive structures is practically completely depressed.

L38 ANSWER 30 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN  
 ACCESSION NUMBER: 1965:480952 HCAPLUS  
 DOCUMENT NUMBER: 63:80952  
 ORIGINAL REFERENCE NO.: 63:14970h,14971a-b  
 TITLE: Monoalkylated glycine derivatives  
 AUTHOR(S): Hanke, H.  
 CORPORATE SOURCE: Univ. Jena, GA

SOURCE: Pharmazeutische Zentralhalle fuer Deutschland (1960), 99(June), 318-22  
From: CZ 1963(26), 10820-1.  
CODEN: PHZEAD; ISSN: 0369-9773

DOCUMENT TYPE: Journal  
LANGUAGE: German

IT 542-53-0, Glycine, N-ethyl-, hydrochloride 627-01-0,  
Glycine, N-ethyl- 3182-81-8, Glycine, N-butyl- 3182-82-9  
, Glycine, N-butyl-, hydrochloride 3182-85-2, Glycine,  
N-isobutyl- 3182-86-3, Glycine, N-isobutyl-, hydrochloride  
3182-89-6, Glycine, N-isohexyl- 3182-90-9, Glycine,  
N-isohexyl-, hydrochloride 3183-21-9, Glycine, N-isopropyl-  
3183-22-0, Glycine, N-isopropyl-, ethyl ester 3183-23-1,  
Glycine, N-isopropyl-, ethyl ester, hydrochloride 3338-22-5,  
Glycine, N-isopropyl-, hydrochloride  
(preparation of)

RN 542-53-0 HCAPLUS  
CN Glycine, N-ethyl-, hydrochloride (7CI, 8CI, 9CI) (CA INDEX NAME)

EtNH-CH<sub>2</sub>-CO<sub>2</sub>H

● HCl

RN 627-01-0 HCAPLUS  
CN Glycine, N-ethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

EtNH-CH<sub>2</sub>-CO<sub>2</sub>H

RN 3182-81-8 HCAPLUS  
CN Glycine, N-butyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

n-BuNH-CH<sub>2</sub>-CO<sub>2</sub>H

RN 3182-82-9 HCAPLUS  
CN Glycine, N-butyl-, hydrochloride (7CI, 8CI, 9CI) (CA INDEX NAME)

n-BuNH-CH<sub>2</sub>-CO<sub>2</sub>H

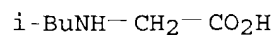
● HCl

RN 3182-85-2 HCAPLUS  
CN Glycine, N-(2-methylpropyl)- (9CI) (CA INDEX NAME)

i-BuNH-CH<sub>2</sub>-CO<sub>2</sub>H

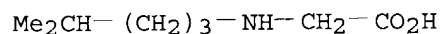
RN 3182-86-3 HCAPLUS

CN Glycine, N-(2-methylpropyl)-, hydrochloride (9CI) (CA INDEX NAME)

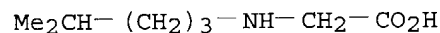


● HCl

RN 3182-89-6 HCAPLUS  
CN Glycine, N-isohexyl- (7CI, 8CI) (CA INDEX NAME)

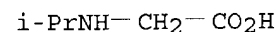


RN 3182-90-9 HCAPLUS  
CN Glycine, N-isohexyl-, hydrochloride (7CI, 8CI) (CA INDEX NAME)

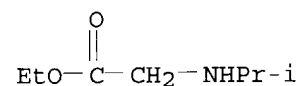


● HCl

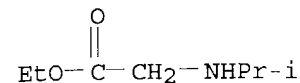
RN 3183-21-9 HCAPLUS  
CN Glycine, N-(1-methylethyl)- (9CI) (CA INDEX NAME)



RN 3183-22-0 HCAPLUS  
CN Glycine, N-(1-methylethyl)-, ethyl ester (9CI) (CA INDEX NAME)



RN 3183-23-1 HCAPLUS  
CN Glycine, N-(1-methylethyl)-, ethyl ester, hydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 3338-22-5 HCAPLUS  
CN Glycine, N-(1-methylethyl)-, hydrochloride (9CI) (CA INDEX NAME)

i-PrNH-CH<sub>2</sub>-CO<sub>2</sub>H

● HCl

AB Primary amine HCl salts with HCHO and KCN yield alkylamino-acetonitriles which can be hydrolyzed with alc. HCl to N-alkylglycines Et ester HCl salts. These treated with NH<sub>3</sub>-CHCl<sub>3</sub> yield the free esters which are converted by acid saponification to the alkylglycine (Ia) and their HCl salts. Thus, to obtain N-ethylglycine (I), m. 180-2° (decomposition), I.HCl is treated with AgOH in water, the mixture filtered, the filtrate gassed with H<sub>2</sub>S, filtered, concentrated, and the residue dissolved in EtOH-Et<sub>2</sub>O. I.HCl m. 179-80°, is prepared by boiling 3 hrs. the Et ester (II) in 6N HCl, evaporating, and dissolving in EtOH-Et<sub>2</sub>O. To prepare II.HCl, m. 135°, HCHO, EtNH<sub>2</sub>.HCl, and KCN are allowed to react 30 min. in aqueous solution at 5° under CO<sub>2</sub>, the mixture kept several hrs., the nitrile formed extracted with Et<sub>2</sub>O (yield 90-100%), boiled 4 hrs. with ethanolic HCl, the NH<sub>4</sub>Cl filtered off and the filtrate concentrated; yield 90-100%. II, b16 58°, is obtained by 30-min. reaction of II.HCl and NH<sub>3</sub>-CHCl<sub>3</sub> at 0° filtering and distilling; yield 55-75%. Similarly were prepared the following Ia (alkyl, m.p., m.p. HCl salt, b.p. Et ester, and m.p. Et ester HCl salt given): isopropyl, 193-5° (decomposition), 202-3°, b2-3 32-5°, 113-15° (decomposition); allyl, 158-9° (decomposition), 167-9° (decomposition), b3 47°, 113-14° (decomposition) (EtOH); n-butyl, 190-1° (decomposition), 202-4°, b2-3 47-51°, 164-6°; isobutyl, 192-3° (decomposition), 210-12° (decomposition) or 221-222° (in sealed tube), b3 49-51°, 127-8.5° (decomposition); isohexyl, 194-5°, 186-7° b4 79°, 182-3°.

L38 ANSWER 31 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1963:435 HCAPLUS

DOCUMENT NUMBER: 58:435

ORIGINAL REFERENCE NO.: 58:63e

TITLE: Physicochemical analysis of isopropylamine-ethyl monochloroacetate system

AUTHOR(S): Bekturov, E. A.

SOURCE: Izvestiya Akademii Nauk Kazakhskoi SSR, Seriya Khimicheskaya (1962), (1), 44-8  
CODEN: IKAKAK; ISSN: 0002-3205

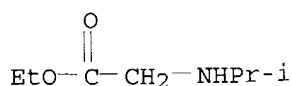
DOCUMENT TYPE: Journal

LANGUAGE: Russian

IT 3183-22-0, Glycine, N-isopropyl-, ethyl ester 3183-23-1,  
Glycine, N-isopropyl-, ethyl ester, hydrochloride  
(formation of)

RN 3183-22-0 HCAPLUS

CN Glycine, N-(1-methylethyl)-, ethyl ester (9CI) (CA INDEX NAME)

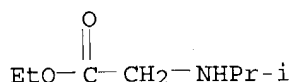


RN 3183-23-1 HCAPLUS

CN Glycine, N-(1-methylethyl)-, ethyl ester, hydrochloride (9CI) (CA INDEX



NAME)



● HCl

AB Measurement of viscosity, d., and conductivity of system  $\text{Me}_2\text{CHNH}_2 + \text{CH}_2\text{-ClCO}_2\text{Et}$  shows the formation of  $(\text{Me}_2\text{CHNH}_2\text{CH}_2\text{CO}_2\text{Et})^+ \cdot \text{Cl}^-$ , which then reacts with the 2nd mol. of amine to form  $\text{Me}_2\text{CHNHCH}_2\text{CO}_2\text{Et}$  and  $\text{Me}_2\text{CHNH}_3\text{Cl}$ .

L38 ANSWER 32 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1956:52502 HCAPLUS

DOCUMENT NUMBER: 50:52502

ORIGINAL REFERENCE NO.: 50:10024h-i,10025a-d

TITLE: The preparation of substituted hydrazines. III. A general method for preparing N-substituted glycines

AUTHOR(S): Tien, Jack M.; Hunsberger, I. Moyer

CORPORATE SOURCE: Antioch Coll., Yellow Springs, O.

SOURCE: Journal of the American Chemical Society (1955

), 77, 6696-8

CODEN: JACSAT; ISSN: 0002-7863

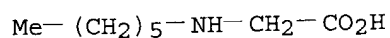
DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

IT 56676-69-8, Glycine, N-hexyl-, hydrochloride  
(preparation of)

RN 56676-69-8 HCAPLUS

CN Glycine, N-hexyl-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

AB cf. C.A. 50, 3431c.  $\text{C}_6\text{H}_{13}\text{NH}_2$  (0.765 g.) and 1.7 g.  $\text{HOCH}_2\text{CO}_2\text{Et}$  (62% pure) in 10 cc. glacial  $\text{AcOH}$  allowed to stand 2 hrs., hydrogenated with shaking 2 hrs. at room temperature and 3-4 atmospheric pressure over 0.1 g. 10%  $\text{Pd-C}$ , the colorless filtrate neutralized with solid  $\text{NaHCO}_3$  and extracted with two 60-cc. portions  $\text{Et}_2\text{O}$ , the residue from the extract refluxed 10 min. with 5 cc. 10% aqueous  $\text{NaOH}$ , cooled, and acidified with 2-3 cc. concentrated  $\text{HCl}$ , and the precipitated small, nearly white plates, m.  $200-6^\circ$ , heated with 25 cc. glacial  $\text{AcOH}$  on a steam bath, filtered hot, and cooled gave 0.4 g. N-hexylglycine (I)  $\text{HCl}$  salt, white flakes, m.  $215-18^\circ$ . The filtrate from the hydrogenation basified with dilute aqueous  $\text{NaOH}$ , refluxed cooled, acidified with excess concentrated  $\text{HCl}$ , and evaporated to dryness, and the residue extracted with hot glacial  $\text{AcOH}$  gave I. $\text{HCl}$ .  $\text{C}_6\text{H}_{13}\text{NH}_2$  and  $\text{HOCH}_2\text{CO}_2\text{Et}$  in 2:3 concentrated  $\text{HCl-H}_2\text{O}$  gave only a very low yield of I. $\text{HCl}$ ; no I. $\text{HCl}$  was detected from a hydrogenation in 6N  $\text{HCl}$ .  $\text{PhNH}_2$  (1.00 g.) in 5 cc. 95%  $\text{EtOH}$  and 1.70 g.

HOCH<sub>2</sub>CO<sub>2</sub>Et (62% pure) hydrogenated 2.5 hrs. and filtered, the catalyst washed with 10 cc. 95% EtOH, and the combined filtrate and washings diluted to the cloud point with H<sub>2</sub>O and cooled gave 1.06 g. N-phenylglycine Et ester (II), white plates, m. 57-8°; 2nd and 3rd crops, 0.41 and 0.17 g., resp. II (0.179 g.) refluxed 10 min. with 2 cc. concentrated HCl and

4 cc. H<sub>2</sub>O and evaporated to dryness in vacuo, the white residue dissolved with warming with 2 cc. concentrated HCl on the steam bath, and the solution cooled gave

0.116 g. N-phenylglycine-HCl salt, m. 172-4°; 2nd crop, 0.041 g. Com. N-phenylglycine (0.1 g.), yellow powder, and 0.1 g. NaCl dissolved at about 70° in 5 cc. H<sub>2</sub>O, and the solution cooled deposited after about 2 min. large pale-yellow needles; a similar recrystn. in the presence of 0.5 cc. AcOH gave colorless crystals, m. 126-7°; the free base dissolved with heating in concentrated HCl on the steam bath, decolorized, and cooled deposited the HCl salt, colorless transparent plates, m. 168-73°; turned lemon-yellow after several days.

L38 ANSWER 33 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1956:12242 HCAPLUS

DOCUMENT NUMBER: 50:12242

ORIGINAL REFERENCE NO.: 50:2534d-i, 2535a-i, 2536a-b

TITLE: The preparation of substituted hydrazines. I. Alkylhydrazines via alkylsydnones

AUTHOR(S): Fugger, Joseph; Tien, Jack M.; Hunsberger, I. Moyer

CORPORATE SOURCE: Antioch Coll., Yellow Springs, O.

SOURCE: Journal of the American Chemical Society (1955), 77, 1843-8

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

OTHER SOURCE(S): CASREACT 50:12242

IT 3182-82-9, Glycine, N-butyl-, hydrochloride 56676-69-8, Glycine, N-hexyl-, hydrochloride (preparation of)

RN 3182-82-9 HCAPLUS

CN Glycine, N-butyl-, hydrochloride (7CI, 8CI, 9CI) (CA INDEX NAME)

n-BuNH-CH<sub>2</sub>-CO<sub>2</sub>H

● HCl

RN 56676-69-8 HCAPLUS

CN Glycine, N-hexyl-, hydrochloride (9CI) (CA INDEX NAME)

Me-(CH<sub>2</sub>)<sub>5</sub>-NH-CH<sub>2</sub>-CO<sub>2</sub>H

● HCl

AB The conversion of an alkylamine to an alkylhydrazine via the corresponding N-alkylglycine, N-nitroso-N-alkylglycine, and N-alkylsydnone is shown to constitute an acceptable preparative method in the cases of PhCH<sub>2</sub>NHNNH<sub>2</sub>

(I), BuNHNH<sub>2</sub> (II), and C<sub>6</sub>H<sub>13</sub>NHNH<sub>2</sub> (III). The infrared spectra of N-benzylsydnone (IV), N-butylsydnone (V), and N-hexylsydnone (VI) are presented. ClCH<sub>2</sub>CO<sub>2</sub>Et (122 g.) and 214 g. PhCH<sub>2</sub>NH<sub>2</sub> in 1 l. C<sub>6</sub>H<sub>6</sub> refluxed 5 hrs. with stirring, the mixture filtered, the filtrate distilled to leave 154 g. PhCH<sub>2</sub>NHCH<sub>2</sub>CO<sub>2</sub>Et, yellow oil, the residue filtered, the crude ester added dropwise with stirring during 15 min. to 63.6 g. NaOH in 300 cc. H<sub>2</sub>O, the yellow solution refluxed 45 min. washed with Et<sub>2</sub>O, and acidified with concentrated HCl to pH 2, the resulting white suspension of PhCH<sub>2</sub>NHCH<sub>2</sub>CO<sub>2</sub>H treated at 0° with stirring during 0.5 hr. with 55.2 g. NaNO<sub>2</sub> in 100 cc. cold H<sub>2</sub>O, the mixture stirred 2 hrs., brought to pH 2 with concentrated HCl, refrigerated 1 hr., and filtered, and the filter residue dried in vacuo over KOH yielded 139 g. crude PhCH<sub>2</sub>N(NO)CH<sub>2</sub>CO<sub>2</sub>H (VII). The VII heated 5 hrs. with stirring on the steam bath with 685 cc. Ac<sub>2</sub>O, the resulting dark red solution filtered, and the filtrate evaporated in vacuo yielded 115 g. crude IV, red-brown oil, which solidified in an ice bath on scratching. The crude IV heated 4.5 hrs. on a steam bath with 1 l. 1:1 HCl, the red solution filtered, the clear filtrate concentrated to less than

100

cc. and filtered, and the residual crude I.HCl (56.8 g.) recrystd. twice from boiling EtOH yielded 14.6 g. pure I.HCl, m. 108-10.5°; and from mother liquor an addnl. 6.1 g. I.HCl. BrCH<sub>2</sub>CO<sub>2</sub>Et (68 cc.) in 100 cc. C<sub>6</sub>H<sub>6</sub> added portionwise with swirling and cooling to 120 cc. BuNH<sub>2</sub> in 300 cc., the mixture refluxed 2 hrs. on a steam bath, cooled, and filtered, the residual HBr salt (59 g.) washed with 80 cc. C<sub>6</sub>H<sub>6</sub>, the combined filtrate and washing concentrated in vacuo until white fumes appeared, the residue refluxed 25 min. with 28 g. NaOH in 120 cc. H<sub>2</sub>O, the cooled alkaline solution extracted with Et<sub>2</sub>O, the aqueous layer acidified with cooling to pH 2 with concentrated

HCl, and the mixture refrigerated and concentrated consecutively yielded 68.9 g.

crude BuNHCH<sub>2</sub>CO<sub>2</sub>H.HCl (VIII).HCl, snow-white needles and plates. Crude VIII.HCl (1 g.) in 10 cc. concentrated HCl warmed slightly on the steam bath

and

filtered, the filtrate refrigerated, and this process repeated 3 times gave pure VIII.HCl, m. 204-5°. C<sub>6</sub>H<sub>13</sub>NH<sub>2</sub> and BrCH<sub>2</sub>CO<sub>2</sub>Et gave in exactly the same manner crude C<sub>6</sub>H<sub>13</sub>NHCH<sub>2</sub>CO<sub>2</sub>H.HCl (IX.HCl); the alkaline

solution

of the IX.HCl swirled with cooling with 90 cc. concentrated HCl and 100 g. chopped ice precipitated immediately 81.0 g. IX.HCl, tiny yellowish white flakes;

refrigeration of the mother liquor gave an addnl. 4.8 g. IX.HCl. Crude IX.HCl (1 g.) in 10 cc. H<sub>2</sub>O treated with 1 cc. concentrated HCl, and the resulting precipitate treated 3 times in the same manner gave pure IX.HCl, snow-white flakes, m. 210-17°. Crude IX.HCl (1 g.) recrystd. from 20 cc. 1:1 MeOH-Me<sub>2</sub>CO or 40 cc. glacial AcOH gave the pure salt. VIII.HCl (78.0 g.) in 300 cc. H<sub>2</sub>O treated during 0.5 hr. at -4 to -5° with 37.5 g. NaNO<sub>2</sub> in 100 cc. H<sub>2</sub>O, the mixture stirred 2 hrs., the oily bottom layer drawn off and dissolved in Et<sub>2</sub>O, and the solution filtered, dried, and evaporated gave 62.0 g. crude BuN(NO)CH<sub>2</sub>CO<sub>2</sub>H (X), yellow granular powder. Crude X (8.0 g.) crystallized from a small amount Et<sub>2</sub>O gave 4.53 g. nearly

white

granular solid, m. 60-2°, which recrystd. from aqueous EtOH or Et<sub>2</sub>O-petr. ether gave pure X, long snow-white flakes, m. 61-2°. An alkaline solution of IX prepared from 0.60 mole BrCH<sub>2</sub>CO<sub>2</sub>Et, cooled, treated

with

stirring with 49.7 g. NaNO<sub>2</sub> in 100 cc. H<sub>2</sub>O in 1 portion followed dropwise during 1.25 hrs. by 90 cc. concentrated HCl diluted with 50 g. ice, stirred 1

hr.,

and adjusted with concentrated HCl to pH 2.0, the resulting brown oily top

layer

of crude  $\text{C}_6\text{H}_{13}\text{N}(\text{NO})\text{CH}_2\text{CO}_2\text{H}$  (XI), (74.8 g.) allowed to stand, and the solidified yellow granular powder recrystd. from Et<sub>2</sub>O and then aqueous EtOH or petr. ether-Et<sub>2</sub>O gave pure XI, long white flakes, m. 79-80°. Crude X (40 g.) in 236 cc. Ac<sub>2</sub>O heated 3 hrs. on the steam bath, the mixture kept 1 day at room temperature, and the excess Ac<sub>2</sub>O distilled off gave 33 g. crude V; an 8-g. sample distilled yielded 4.5 g. pure V, pale yellow oil, b<sub>2</sub> 165-7°. X (0.362 mole) heated 3 hrs. with only 1.09 moles Ac<sub>2</sub>O gave nearly identical results. Crude yellow-white XI prepared from 0.20 mole  $\text{BrCH}_2\text{CO}_2\text{Et}$  dissolved in Et<sub>2</sub>O, the extract dried over Na<sub>2</sub>SO<sub>4</sub>, treated with 190 cc. Ac<sub>2</sub>O, kept 1 day at room temperature, and evaporated on the steam bath, the residual oil refluxed 3 hrs., the excess Ac<sub>2</sub>O removed in vacuo, and the clear brown oil dried in vacuo over KOH and P<sub>2</sub>O<sub>5</sub> yielded 23 g. crude VI, which on distillation yielded 18 g. pure VI, b<sub>0.43</sub> 170-6° (redistd., b<sub>0.09</sub> 141-3°). XI (0.334 mole) dissolved in 1.14 moles warm AcOH, and the brown solution heated 2 hrs. on the steam bath after standing overnight yielded 93% VI. Crude V (40.5 g.) mixed with 80 cc. concentrated HCl, the mixture heated 2 hrs. on the steam bath, cooled to room temperature, treated with 20 cc. concentrated HCl, refrigerated overnight, treated with dry HCl to beginning crystallization, refrigerated again, and filtered, the residue washed with 1:1 MeOH-Et<sub>2</sub>O to yield 22 g. nearly white transparent needles, the filtrate decolorized with Norit A, saturated below 0° with dry HCl, refrigerated several days, neutralized with solid Na<sub>2</sub>CO<sub>3</sub>, and extracted with Et<sub>2</sub>O, a part of the extract treated with dry HCl, and the white precipitate filtered off gave II.HCl; the remainder of the extract treated in EtOH with (CO<sub>2</sub>H)<sub>2</sub> yielded the oxalate of II. Distilled V (4.4 g.) heated 2.5 hrs. with concentrated HCl, the yellow solution treated after 2 hrs. with an addnl. 10 cc. HCl, and the solution cooled and saturated with dry HCl yielded 3.1 g. II.HCl, thin white plates, m. 149-54°. II.HCl (3.0 g.) treated with 15 cc. 25% aqueous Na<sub>2</sub>CO<sub>3</sub>, the alkaline mixture extracted with Et<sub>2</sub>O, and the extract distilled gave 1.0 g. V, colorless liquid with an amine odor, b<sub>20</sub> 82-5°. Crude VI.HCl (40.7 g.) and 80 cc. concentrated HCl heated 2 hrs. on the steam bath, the mixture treated with an addnl. 30 cc. HCl and refrigerated, the dark brown cake dissolved in about 150 cc. H<sub>2</sub>O, and the solution heated a few min. on the steam bath with about 5 g. Norit, filtered hot, and cooled deposited 19.8 g. III.HCl, fine transparent needles; the mother liquor treated with (CO<sub>2</sub>H)<sub>2</sub> in EtOH gave 18.0 g. III oxalate. The alkaline solution of the Na salt of IX from 0.60 mole  $\text{BrCH}_2\text{CO}_2\text{Et}$  treated below 0° with 37.2 g. NaNO<sub>2</sub> in 120 cc. H<sub>2</sub>O in 1 portion, the mixture allowed to stand 0.5 hr., treated with 100 cc. concentrated HCl containing 50 g. crushed ice, stirred 1 hr., and extracted with Et<sub>2</sub>O, and the Et<sub>2</sub>O evaporated gave a residue of 88.7 g. XI. XI (83.7 g.) heated 2 hrs. on the steam bath with 126 cc. Ac<sub>2</sub>O, the excess Ac<sub>2</sub>O removed gave 81.5 g. crude VI. Crude VI (64 g.) heated 2 hrs. on a steam bath with 110 cc. concentrated HCl, cooled, neutralized with 25% aqueous NaOH, saturated with K<sub>2</sub>CO<sub>3</sub>, and extracted 8 times with Et<sub>2</sub>O, the extract dried with K<sub>2</sub>CO, and added to 76 g. (CO<sub>2</sub>H)<sub>2</sub> in 400 cc. 95% EtOH, the mixture allowed to stand overnight, and the yellowish solid filtered off and dried yielded 55.5 g. crude III.(CO<sub>2</sub>H)<sub>2</sub>. Crude III.(CO<sub>2</sub>H)<sub>2</sub> (1.0 g.) recrystd. from 25 cc. hot 9:1 MeOH-EtOH yielded 410 mg. fluffy flakes, m. 171-2°; a 94-mg. sample in 5 cc. hot MeOH evaporated slowly at room temperature yielded 64 mg. large white

needles, m. 173-3.5°; this material dissolved in 5 cc. hot 4; 1 MeOH-EtOH, the solution filtered, and the filtrate poured into a sintered glass funnel gave 26 mg. pure III.(CO<sub>2</sub>H)<sub>2</sub>, transparent needles, m. 174.5-5.5°. II.HCl dissolved in 150-200 cc. H<sub>2</sub>O, neutralized with 30% aqueous NaOH in portions, saturated with solid K<sub>2</sub>CO<sub>3</sub>, and extracted with Et<sub>2</sub>O, the extract dried over K<sub>2</sub>CO<sub>3</sub> and added to 54 g. (CO<sub>2</sub>H)<sub>2</sub> in 320 cc. 95% EtOH, the mixture allowed to stand overnight and filtered to give 18.5 g. crude salt, the mother liquor of the original II.HCl treated in the same manner to give an addnl. 6.3 g. oxalate, and the solid material combined gave 24.8 g. crude II.(CO<sub>2</sub>H)<sub>2</sub>. Crude II.(CO<sub>2</sub>H)<sub>2</sub> (1 g.) recrystd. from 60 cc. hot 9:1 MeOH-EtOH yielded 420 mg. pure material, fine snow white needles; a sample (180 mg.) recrystd. from 20 cc. of the same solvent yielded 144 mg. pure material, white needles, m. 164-5°.

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FILE COVERS 1907 - 3 Jun 2004 VOL 140 ISS 23  
FILE LAST UPDATED: 2 Jun 2004 (20040602/ED)

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FILE COVERS 1907 - 3 Jun 2004 VOL 140 ISS 23  
 FILE LAST UPDATED: 2 Jun 2004 (20040602/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=&gt; FIL STNGUIDE

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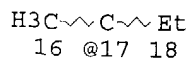
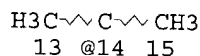
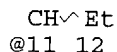
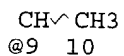
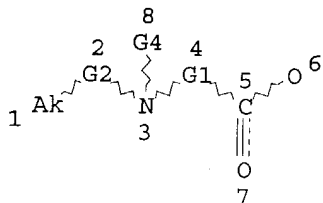
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*R<sub>1</sub> = unsubstituted  
alkyl group*

=&gt; d que 138

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 DYCK, L? AND LIU, Y? AND BOULTON, A? AND PATERSON, I?)/AU  
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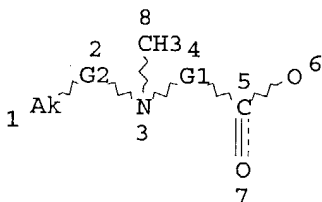
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application


$$\text{CH} \sim \text{CH}_3$$

@9 10

CH $\searrow$ Et  
@11 12

$$\text{H3C} \sim \text{C} \sim \text{CH3}$$

13 @14 15

$$\begin{array}{c} \text{H3C} \sim \text{C} \sim \text{Et} \\ 16 \quad @17 \quad 18 \end{array}$$

```

REP G1=(1-3) CH2
VAR G2=CH2/9/11/14/17
NODE ATTRIBUTES:
CONNECT IS E1 RC AT 1
CONNECT IS E3 RC AT 3
CONNECT IS E1 RC AT 6
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED
ECOUNT IS M1-X17 C AT 1

```

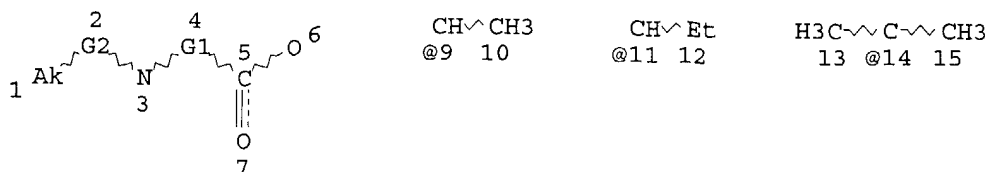
GRAPH ATTRIBUTES:  
RING(S) ARE ISOLATED OR EMBEDDED  
NUMBER OF NODES IS 18

STEREO ATTRIBUTES: NONE



L18

STR



H3C~C~Et  
16 @17 18

REP G1=(1-3) CH2  
VAR G2=CH2/9/11/14/17  
NODE ATTRIBUTES:  
CONNECT IS E1 RC AT 1  
CONNECT IS E2 RC AT 3  
CONNECT IS E1 RC AT 6  
DEFAULT MLEVEL IS ATOM  
DEFAULT ECLEVEL IS LIMITED  
ECOUNT IS M1-X17 C AT 1

GRAPH ATTRIBUTES:  
RING(S) ARE ISOLATED OR EMBEDDED  
NUMBER OF NODES IS 17

STEREO ATTRIBUTES: NONE

L19 ( 295)SEA FILE=REGISTRY SUB=L11 SSS FULL (L17 OR L18)  
L20 ( 976)SEA FILE=HCAPLUS ABB=ON ~~PLU=ON~~ L19  
L21 ( 5)SEA FILE=REGISTRY ABB=ON PLU=ON (58482-93-2 OR 42313-51-9 OR 3338-22-5 OR 3183-22-0 OR 3183-21-9)/RN  
L22 ( 36)SEA FILE=REGISTRY ABB=ON PLU=ON L16 NOT L21  
L23 ( 34)SEA FILE=HCAPLUS ABB=ON PLU=ON L22  
L24 ( 28)SEA FILE=HCAPLUS ABB=ON PLU=ON L23 AND (PY<1999 OR AY<1999 OR PRY<1999)  
L25 ( 83)SEA FILE=HCAPLUS ABB=ON PLU=ON L21  
L26 ( 5)SEA FILE=HCAPLUS ABB=ON PLU=ON L24 AND L25  
L27 ( 28)SEA FILE=HCAPLUS ABB=ON PLU=ON L26 OR L24  
L28 ( 24)SEA FILE=HCAPLUS ABB=ON PLU=ON L20 AND L27  
L29 28 SEA FILE=HCAPLUS ABB=ON PLU=ON L27 OR L28  
L32 5 SEA FILE=HCAPLUS ABB=ON PLU=ON (58482-93-2? OR 42313-51-9?) (L) (BIOL OR USES)/RL  
L33 5 SEA FILE=HCAPLUS ABB=ON PLU=ON L32 AND (PY<1999 OR AY<1999 OR PRY<1999)  
L34 14 SEA FILE=HCAPLUS ABB=ON PLU=ON 42313-51-9?  
L35 14 SEA FILE=HCAPLUS ABB=ON PLU=ON L34 AND (PY<1999 OR AY<1999 OR PRY<1999)  
L37 1 SEA FILE=HCAPLUS ABB=ON PLU=ON L35 AND (A61K?)/ICM  
L38 33 SEA FILE=HCAPLUS ABB=ON PLU=ON L37 OR L33 OR L29

*remove quaternary  
N<sup>+</sup> salts*

=&gt;

=&gt; d l38 ibib hitstr abs

YOU HAVE REQUESTED DATA FROM FILE 'HCAPLUS' - CONTINUE? (Y)/N:y

L38 ANSWER 1 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1999:626163 HCAPLUS  
 DOCUMENT NUMBER: 131:243589  
 TITLE: Aliphatic amino carboxylic and amino  
 amino nitriles, and amino tetrazole  
 rescue agents *Applicants*  
 INVENTOR(S): Paterson, I. Alick; Dyck, Lilian E.,  
 Liu, Ya-Dong; Durden, David A.; Boul  
 PATENT ASSIGNEE(S): University of Saskatchewan Technolog  
 The Canada Trust Company  
 SOURCE: PCT Int. Appl., 52 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9948858	A2	19990930	WO 1999-CA250	19990325 <--
WO 9948858	A3	20000120		
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2325943	AA	19990930	CA 1999-2325943	19990325 <--
AU 9928240	A1	19991018	AU 1999-28240	19990325 <--
AU 767098	B2	20031030		
TR 200002756	T2	20001221	TR 2000-200002756	19990325 <--
EP 1064254	A2	20010103	EP 1999-908728	19990325 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
BR 9909103	A	20011016	BR 1999-9103	19990325 <--
JP 2002507591	T2	20020312	JP 2000-537843	19990325 <--
ZA 2000004988	A	20010507	ZA 2000-4988	20000919 <--
NO 2000004774	A	20000925	NO 2000-4774	20000925 <--
PRIORITY APPLN. INFO.:			US 1998-79488P	P 19980326 <--
			US 1998-79489P	P 19980326 <--
			WO 1999-CA250	W 19990325

OTHER SOURCE(S): MARPAT 131:243589

IT 3338-22-5P 31044-48-1P 41331-11-7P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological  
 study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU  
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT  
 (Reactant or reagent); USES (Uses)

(preparation of aliphatic amino carboxylic and amino phosphonic acids, amino  
 nitriles, and amino tetrazoles as cellular rescue agents)

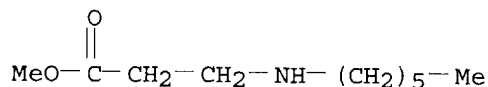
RN 3338-22-5 HCAPLUS

CN Glycine, N-(1-methylethyl)-, hydrochloride (9CI) (CA INDEX NAME)

i-PrNH-CH<sub>2</sub>-CO<sub>2</sub>H

● HCl

RN 31044-48-1 HCAPLUS  
CN β-Alanine, N-hexyl-, methyl ester, hydrochloride (8CI, 9CI) (CA INDEX NAME)



● HCl

RN 41331-11-7 HCAPLUS  
CN β-Alanine, N-hexyl- (9CI) (CA INDEX NAME)

Me-(CH<sub>2</sub>)<sub>5</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-CO<sub>2</sub>H

IT 3183-21-9P 3183-22-0P 3183-23-1P  
16217-35-9P 27453-30-1P 31044-47-0P  
40870-77-7P 41331-10-6P 42313-51-9P  
56676-69-8P 244189-67-1P 244189-68-2P  
244189-69-3P 244189-70-6P 244189-71-7P  
244189-72-8P 244189-73-9P 244189-74-0P  
244189-75-1P 244189-98-8P 244189-99-9P  
244190-00-9P 244190-01-0P 244190-02-1P  
244190-03-2P 244190-04-3P 244190-26-9P  
244190-27-0P 244190-28-1P 244190-31-6P  
244190-32-7P 244190-33-8P 244190-34-9P  
244190-37-2P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);

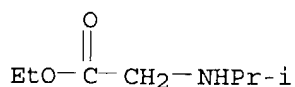
**BIOL (Biological study); PREP (Preparation); USES (Uses)**

(preparation of aliphatic amino carboxylic and amino phosphonic acids, amino nitriles, and amino tetrazoles as cellular rescue agents)

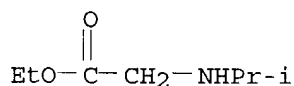
RN 3183-21-9 HCAPLUS  
CN Glycine, N-(1-methylethyl)- (9CI) (CA INDEX NAME)

i-PrNH-CH<sub>2</sub>-CO<sub>2</sub>H

RN 3183-22-0 HCAPLUS  
CN Glycine, N-(1-methylethyl)-, ethyl ester (9CI) (CA INDEX NAME)

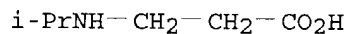


RN 3183-23-1 HCAPLUS  
 CN Glycine, N-(1-methylethyl)-, ethyl ester, hydrochloride (9CI) (CA INDEX NAME)

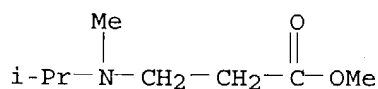


● HCl

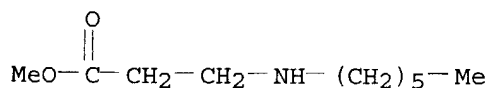
RN 16217-35-9 HCAPLUS  
 CN  $\beta$ -Alanine, N-(1-methylethyl)- (9CI) (CA INDEX NAME)



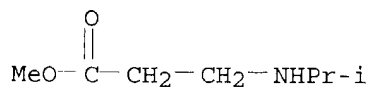
RN 27453-30-1 HCAPLUS  
 CN  $\beta$ -Alanine, N-methyl-N-(1-methylethyl)-, methyl ester (9CI) (CA INDEX NAME)



RN 31044-47-0 HCAPLUS  
 CN  $\beta$ -Alanine, N-hexyl-, methyl ester (8CI, 9CI) (CA INDEX NAME)

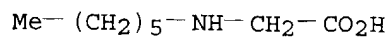


RN 40870-77-7 HCAPLUS  
 CN  $\beta$ -Alanine, N-(1-methylethyl)-, methyl ester, hydrochloride (9CI) (CA INDEX NAME)

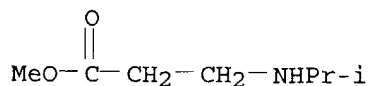


● HCl

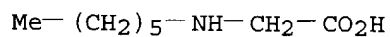
RN 41331-10-6 HCAPLUS  
 CN Glycine, N-hexyl- (9CI) (CA INDEX NAME)



RN 42313-51-9 HCAPLUS  
 CN  $\beta$ -Alanine, N-(1-methylethyl)-, methyl ester (9CI) (CA INDEX NAME)



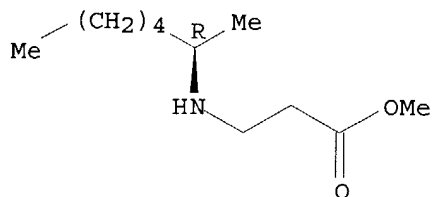
RN 56676-69-8 HCAPLUS  
 CN Glycine, N-hexyl-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 244189-67-1 HCAPLUS  
 CN  $\beta$ -Alanine, N-[(1R)-1-methylhexyl]-, methyl ester, hydrochloride (9CI)  
 (CA INDEX NAME)

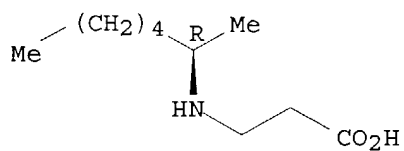
Absolute stereochemistry.



● HCl

RN 244189-68-2 HCAPLUS  
 CN  $\beta$ -Alanine, N-[(1R)-1-methylhexyl]-, hydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

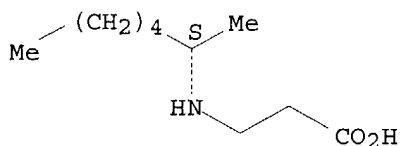


● HCl

RN 244189-69-3 HCAPLUS

CN β-Alanine, N-[(1S)-1-methylhexyl]-, hydrochloride (9CI) (CA INDEX NAME)

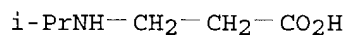
Absolute stereochemistry.



● HCl

RN 244189-70-6 HCAPLUS

CN β-Alanine, N-(1-methylethyl)-, hydrochloride (9CI) (CA INDEX NAME)

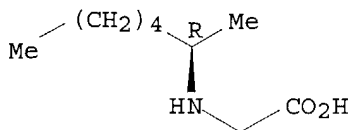


● HCl

RN 244189-71-7 HCAPLUS

CN Glycine, N-[(1R)-1-methylhexyl]-, hydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

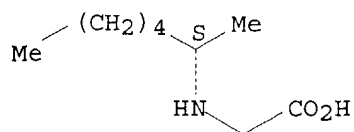


● HCl

RN 244189-72-8 HCAPLUS

CN Glycine, N-[(1S)-1-methylhexyl]-, hydrochloride (9CI) (CA INDEX NAME)

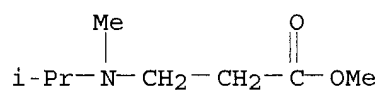
Absolute stereochemistry.



● HCl

RN 244189-73-9 HCAPLUS

CN  $\beta$ -Alanine, N-methyl-N-(1-methylethyl)-, methyl ester, hydrochloride  
(9CI) (CA INDEX NAME)

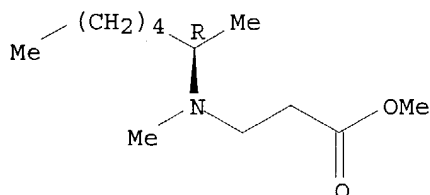


● HCl

RN 244189-74-0 HCAPLUS

CN  $\beta$ -Alanine, N-methyl-N-[(1R)-1-methylhexyl]-, methyl ester,  
hydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

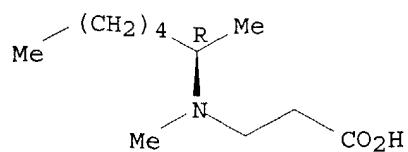


● HCl

RN 244189-75-1 HCAPLUS

CN  $\beta$ -Alanine, N-methyl-N-[(1R)-1-methylhexyl]-, hydrochloride (9CI) (CA  
INDEX NAME)

Absolute stereochemistry.

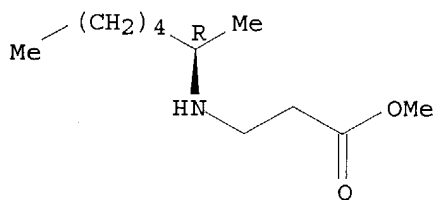


● HCl

RN 244189-98-8 HCAPLUS

CN β-Alanine, N-[(1R)-1-methylhexyl]-, methyl ester (9CI) (CA INDEX NAME)

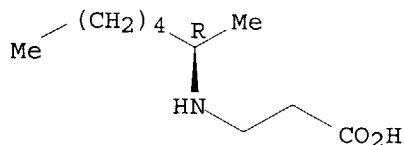
Absolute stereochemistry.



RN 244189-99-9 HCAPLUS

CN β-Alanine, N-[(1R)-1-methylhexyl]- (9CI) (CA INDEX NAME)

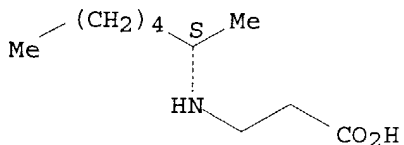
Absolute stereochemistry.



RN 244190-00-9 HCAPLUS

CN β-Alanine, N-[(1S)-1-methylhexyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

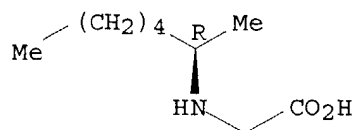


RN 244190-01-0 HCAPLUS

CN Glycine, N-[(1R)-1-methylhexyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

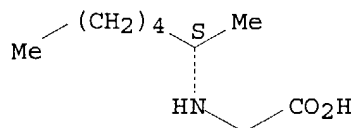




RN 244190-02-1 HCAPLUS

CN Glycine, N-[(1S)-1-methylhexyl]- (9CI) (CA INDEX NAME)

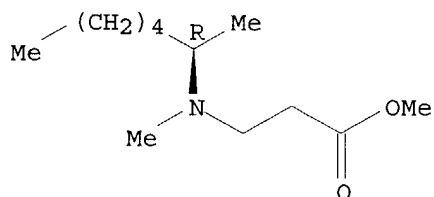
Absolute stereochemistry.



RN 244190-03-2 HCAPLUS

CN  $\beta$ -Alanine, N-methyl-N-[(1R)-1-methylhexyl]-, methyl ester (9CI) (CA INDEX NAME)

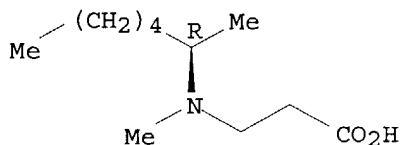
Absolute stereochemistry.



RN 244190-04-3 HCAPLUS

CN  $\beta$ -Alanine, N-methyl-N-[(1R)-1-methylhexyl]- (9CI) (CA INDEX NAME)

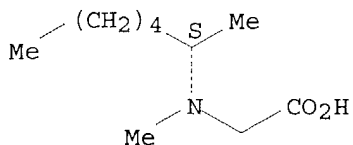
Absolute stereochemistry.



RN 244190-26-9 HCAPLUS

CN Glycine, N-methyl-N-[(1S)-1-methylhexyl]- (9CI) (CA INDEX NAME)

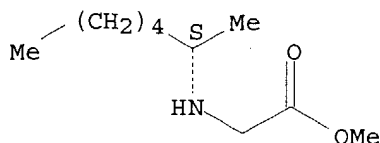
Absolute stereochemistry.



RN 244190-27-0 HCAPLUS

CN Glycine, N-[(1S)-1-methylhexyl]-, methyl ester (9CI) (CA INDEX NAME)

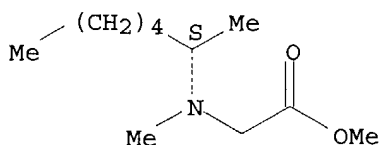
Absolute stereochemistry.



RN 244190-28-1 HCAPLUS

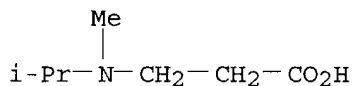
CN Glycine, N-methyl-N-[(1S)-1-methylhexyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



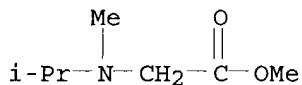
RN 244190-31-6 HCAPLUS

CN  $\beta$ -Alanine, N-methyl-N-(1-methylethyl)- (9CI) (CA INDEX NAME)



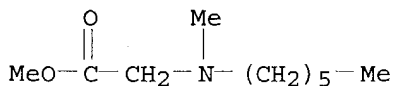
RN 244190-32-7 HCAPLUS

CN Glycine, N-methyl-N-(1-methylethyl)-, methyl ester (9CI) (CA INDEX NAME)



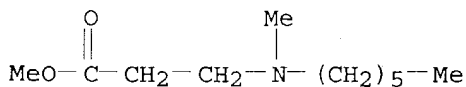
RN 244190-33-8 HCAPLUS

CN Glycine, N-hexyl-N-methyl-, methyl ester (9CI) (CA INDEX NAME)

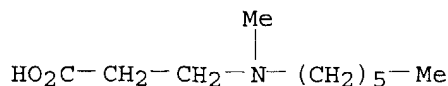


RN 244190-34-9 HCAPLUS

CN  $\beta$ -Alanine, N-hexyl-N-methyl-, methyl ester (9CI) (CA INDEX NAME)



RN 244190-37-2 HCAPLUS  
 CN  $\beta$ -Alanine, N-hexyl-N-methyl- (9CI) (CA INDEX NAME)



AB Tile compds. R1R2R3CNR4(CH2)nX [R1 = Me(CH2)n (n = 1-16), alkenyl, alkynyl, alkoxy, alkylthio, alkylsulfinyl; R2 = H, Me, Et; R3, R4 = H, Me; X = CO2H or carbalkoxy, cyano, PO3H2 or phosphonate ester, 5-tetrazolyl] or their pharmaceutically acceptable salts were prepared. Thus, Me 3-(1-hexylamino)propionate hydrochloride was prepared by addition reaction of 1-hexylamine with Me acrylate and shown to have antiapoptotic activity at 10<sup>-6</sup> M.

=> d 138 ibib hitstr abs 2-

YOU HAVE REQUESTED DATA FROM FILE 'HCAPLUS' - CONTINUE? (Y)/N:y

YOU HAVE REQUESTED DATA FROM 32 ANSWERS - CONTINUE? Y/(N):y

L38 ANSWER 2 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1998:675926 HCAPLUS

DOCUMENT NUMBER: 130:3527

TITLE: Selective addition of amines to methyl acrylate in presence of alumina

AUTHOR(S): Suzuki, Yoshitada; Murakami, Shunsuke; Kodomari, Mitsuo

CORPORATE SOURCE: Department of Industrial Chemistry, Faculty of Engineering, Shibaura Institute of Technology, Minato-ku, Tokyo, 108-8548, Japan

SOURCE: Nippon Kagaku Kaishi (1998), (10), 664-669  
 CODEN: NKAKB8; ISSN: 0369-4577

PUBLISHER: Nippon Kagakkai

DOCUMENT TYPE: Journal

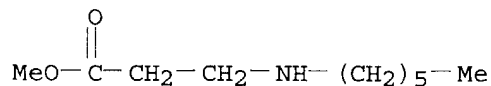
LANGUAGE: Japanese

IT 31044-47-0P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (selective addition of amines to Me acrylate in presence of alumina)

RN 31044-47-0 HCAPLUS

CN  $\beta$ -Alanine, N-hexyl-, methyl ester (8CI, 9CI) (CA INDEX NAME)



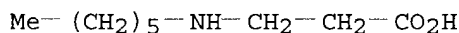
AB The Michael type addition of primary amines to Me acrylate in benzene was accelerated by alumina, and monoadducts were selectively obtained in high yield. The reaction in benzene did not proceed without alumina. The yields of adducts were dependent on the structure of amines; the monoadducts were obtained in high yield (77-91% yield) when linear amines were used, and in the case of branched or bulky primary amines and secondary amines, the yields were decreased compared to the linear ones. In the addition of diamines to Me acrylate, only an amino group on 1 side of the diamines added to Me acrylate to give the monoadducts selectively, and

AB Substituted amines  $R_1NR_2R_3$  [ $R_1$  = acidic group containing at least one OH;  $R_2$  = H, Me,  $PhCH_2$ ,  $R_1$ ,  $R_3$ ;  $R_3$  =  $CR_4R_5CHR_6R_7$ ;  $R_2R_3N$  = heterocyclyl;  $R_4$ ,  $R_5$  = H, C1-6 alkyl, (un)substituted aryl;  $R_6$ ,  $R_7$  =  $R_4$ ,  $R_5$ , OH, C1-6 alkoxy, aryloxy, halo, SH, thioalkyl, mono- or dialkylamino, or, when  $R_6$  = H,  $R_7$  can be  $N(CH_2CO_2H)_2$ ] were dealkylated by heating at 250-400° in aqueous alkali, using at least the stoichiometric amount of alkali needed to neutralize the acidic OH groups, to give  $R_1R_2NH$  with removal of  $R_3$  groups as alkenes. The process is useful for preparation of valuable amino acids, e.g., glycine, sarcosine, iminodiacetic acid, and aminomethylphosphonic acid. Thus, a solution of 0.038 mol  $Me_2CHNMeCH_2CO_2H$  in  $H_2O$  containing 0.076 mol NaOH was heated at 300° in an Monel autoclave to give 71% sarcosine.

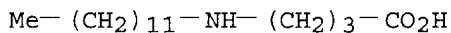
L38 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN  
 ACCESSION NUMBER: 1986:462332 HCAPLUS  
 DOCUMENT NUMBER: 105:62332  
 TITLE: Surface treatment of zinc base materials  
 INVENTOR(S): Kurihara, Masao; Kimata, Shizuro; Imura, Hideaki; Naruse, Naohiko  
 PATENT ASSIGNEE(S): Toa Gosei Chemical Industry Co., Ltd., Japan  
 SOURCE: Jpn. Tokkyo Koho, 9 pp.  
 CODEN: JAXXAD  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 60056225	B4	19851209	JP 1978-102938	19780825 <--
JP 55031417	A2	19800305		

PRIORITY APPLN. INFO.: JP 1978-102938 19780825 <--  
 IT 41331-11-7 41421-76-5  
 RL: USES (Uses)  
 (pretreatment by aqueous alkalies and, of zinc, for coating with powdered epoxy resin)  
 RN 41331-11-7 HCAPLUS  
 CN  $\beta$ -Alanine, N-hexyl- (9CI) (CA INDEX NAME)



RN 41421-76-5 HCAPLUS  
 CN Butanoic acid, 4-(dodecylamino)- (9CI) (CA INDEX NAME)



AB Surfaces of zinc are treated with aqueous alkali hydroxide and aqueous solns. of  $RNHCH_2nCO_2H$  ( $R$  = >C6 saturated or unsatd. aliphatic hydrocarbyl groups,  $n > 2$ ) or H halide solns. and coated. Thus, Zn-plated steel was degreased, treated with 6% aqueous KOH, immersed 5 min at 90° in 3% aqueous hexyl- $\beta$ -aminopropionic acid, dried, electrostatically coated with a powdered epoxy resin, and baked to form a coating.

L38 ANSWER 16 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1986:73067 HCAPLUS  
DOCUMENT NUMBER: 104:73067  
TITLE: Effect of surfactants on the formation of a metallic film during metalizing of glass fibers  
AUTHOR(S): Ermakov, E. A.; Pantaev, V. A.  
CORPORATE SOURCE: Kalinin. Gos. Univ., Kalinin, USSR  
SOURCE: Khim. Poverkh. -Akt. Veshchestv Kompleksonov (1984), 107-10. Editor(s): Gorelov, I. P.  
Kalinin. Gos. Univ.: Kalinin, USSR.  
CODEN: 54JOAA  
DOCUMENT TYPE: Conference  
LANGUAGE: Russian  
IT 41331-11-7  
RL: USES (Uses)  
(surfactant, in electroless copper coating of glass fibers, film d. and structure in relation to)  
RN 41331-11-7 HCAPLUS  
CN  $\beta$ -Alanine, N-hexyl- (9CI) (CA INDEX NAME)

Me- (CH<sub>2</sub>)<sub>5</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-CO<sub>2</sub>H

AB The effect of surfactants, i.e. Na alkylsulfates and alkyl- $\beta$ -alanine on the formation of a metal film during electroless Cu coating of glass fibers was studied. Elec. resistance of the fibers metalized without surfactants was substantially higher than that of samples prepared using the surfactants, which was associated with the difference in the Cu film surface defectiveness. Coatings obtained using the surfactants were distinguished by the fine-crystalline structure, whereas without them, coarser crystallites formed, and the coating was less dense. The best results in preparing dense coatings with fine-grained structure were observed when electroless bath contained Na undecylsulfate [1072-24-8] and N-hexyl- $\beta$ -alanine [41331-11-7].

L38 ANSWER 17 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1986:24719 HCAPLUS  
DOCUMENT NUMBER: 104:24719  
TITLE: Effect of inorganic salts of tin and palladium on colloidal-chemical properties of surfactants  
AUTHOR(S): Voronchikhina, L. I.; Pavlova, L. A.  
CORPORATE SOURCE: Kalinin. Gos. Univ., Kalinin, USSR  
SOURCE: Khim. Poverkh. -Akt. Veshchestv Kompleksonov (1984), 88-92. Editor(s): Gorelov, I. P.  
Kalinin. Gos. Univ.: Kalinin, USSR.  
CODEN: 54JOAA  
DOCUMENT TYPE: Conference  
LANGUAGE: Russian  
IT 41331-11-7  
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)  
(surface activity of, in presence of tin or palladium chlorides)  
RN 41331-11-7 HCAPLUS  
CN  $\beta$ -Alanine, N-hexyl- (9CI) (CA INDEX NAME)

Me- (CH<sub>2</sub>)<sub>5</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-CO<sub>2</sub>H

AB The behavior of colloidal solns. of surfactants (amphoteric

N-dodecyl-N,N-dimethyl- $\alpha$ -betain and N-ketyl- $\beta$ -alanine; anionic Na cetyl sulfate and Na undecyl sulfate and cationic decylpyridinium chloride and dodecylbenzyltrimethylammonium chloride) was studied in the presence of SnCl<sub>2</sub> and PdCl<sub>2</sub>. The saturated adlayer formation, critical micellization concentration, and surface tension were determined At < 0.5M SnCl<sub>2</sub> and PdCl<sub>2</sub> in solns., surface activity of the amphoteric and anionic surfactants increases significantly. The cationic surfactants are unstable in the presence of > 0.05M surfactants.

L38 ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1980:147180 HCAPLUS  
DOCUMENT NUMBER: 92:147180  
TITLE: Cation-binding cyclic peptides with lipophilic tails  
AUTHOR(S): Deber, C. M.; Adawadkar, P. D.  
CORPORATE SOURCE: Res. Inst., Hosp. Sick Child., Toronto, ON, M5G 1X8, Can.  
SOURCE: Biopolymers (1979), 18(10), 2375-96  
CODEN: BIPMAA; ISSN: 0006-3525  
DOCUMENT TYPE: Journal  
LANGUAGE: English

IT 20933-56-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and esterification of, with benzyl alc.)

RN 20933-56-6 HCAPLUS

CN Glycine, N-decyl- (8CI, 9CI) (CA INDEX NAME)

Me- (CH<sub>2</sub>)<sub>9</sub>-NH-CH<sub>2</sub>-CO<sub>2</sub>H

IT 41331-10-6P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 41331-10-6 HCAPLUS

CN Glycine, N-hexyl- (9CI) (CA INDEX NAME)

Me- (CH<sub>2</sub>)<sub>5</sub>-NH-CH<sub>2</sub>-CO<sub>2</sub>H

AB Cyclo[Glu(OCH<sub>2</sub>Ph)-Sar-Gly-NRCH<sub>2</sub>CO]<sub>2</sub> (I; Sar = NMeCH<sub>2</sub>CO, R = Me) was prepared by coupling BOC-Glu(OCH<sub>2</sub>Ph)-Sar-Gly-Sar-OH (BOC = Me<sub>3</sub>CO<sub>2</sub>C) to H-Glu(OCH<sub>2</sub>Ph)-Sar-Gly-Sar-OH by the mixed anhydride method, esterifying the resulting octapeptide with HOC<sub>6</sub>H<sub>4</sub>NO<sub>2</sub>-p, BOC-deblocking the resulting p-nitrophenyl ester with HCl, and cyclizing the resulting H-[Glu(OCH<sub>2</sub>Ph)-Sar-Gly-Sar]<sub>2</sub>-OC<sub>6</sub>H<sub>4</sub>NO<sub>2</sub>-p in DMF/pyridine at high dilution I [R = decyl (II), hexyl, cyclohexyl], cyclo[Glu(OCH<sub>2</sub>Ph)-Sar-Gly-Sar-Glu(OCH<sub>2</sub>Ph)-Sar-Gly-NR<sub>1</sub>CH<sub>2</sub>CO]<sub>2</sub> (R<sub>1</sub> = decyl), and cyclo(Phe-Sar-Gly-Sar)<sub>2</sub> were also prepared, and the above  $\alpha$ -benzyl esters were converted to the free acids. Proton and <sup>13</sup>C NMR data showed that I with a mixture of cis/trans peptide bond conformers were converted to the C<sub>2</sub>-sym. all-trans conformers upon complexation with Ca<sup>2+</sup>. II mediated the transport of cations across a thick-liquid membrane with the following selectivity: Ca<sup>2+</sup> > Na<sup>+</sup> > K<sup>+</sup> > Mn<sup>2+</sup> > Cu<sup>2+</sup> > Mg<sup>2+</sup> > Co<sup>2+</sup> > Zn<sup>2+</sup>.

L38 ANSWER 19 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1977:135270 HCAPLUS

DOCUMENT NUMBER: 86:135270

TITLE: Facilitated diffusion of amino acids across  
bimolecular lipid membranes as a model for selective  
accumulation of amino acids in a primordial protocell

AUTHOR(S): Stillwell, William

CORPORATE SOURCE: Dep. Biophys., Michigan State Univ., East Lansing, MI,  
USA

SOURCE: BioSystems (1976), 8(3), 111-17  
CODEN: BSYMBO; ISSN: 0303-2647

DOCUMENT TYPE: Journal

LANGUAGE: English

IT 627-01-0 3182-81-8 41331-10-6  
50997-13-2

RL: PEP (Physical, engineering or chemical process); PROC (Process)  
(diffusion of, across lipid membrane)

RN 627-01-0 HCAPLUS

CN Glycine, N-ethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

EtNH-CH<sub>2</sub>-CO<sub>2</sub>H

RN 3182-81-8 HCAPLUS

CN Glycine, N-butyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

n-BuNH-CH<sub>2</sub>-CO<sub>2</sub>H

RN 41331-10-6 HCAPLUS

CN Glycine, N-hexyl- (9CI) (CA INDEX NAME)

Me-(CH<sub>2</sub>)<sub>5</sub>-NH-CH<sub>2</sub>-CO<sub>2</sub>H

RN 50997-13-2 HCAPLUS

CN Glycine, N-nonyl- (9CI) (CA INDEX NAME)

Me-(CH<sub>2</sub>)<sub>8</sub>-NH-CH<sub>2</sub>-CO<sub>2</sub>H

AB A simple transport system for the uptake of amino acids into lipid vesicles was studied as a model for the protocell. The rate of diffusion of amino acids across bimol. lipid membranes was greatly stimulated by water-soluble aldehydes. Even HCHO was an effective carrier, although pyridoxal was much more effective. Series of reduced amino acid imines of glycine, lysine, and histidine were synthesized to measure the relative abilities of different aldehydes as carriers for amino acids. Comparison of partition coeffs. to the diffusion rates of the derivatized amino acids indicated that the more lipophilic derivs. are more readily diffused. This simple type of facilitated diffusion makes lipid vesicles an attractive model of the 1st primordial cell.

L38 ANSWER 20 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1976:430029 HCAPLUS

DOCUMENT NUMBER: 85:30029

TITLE: Oxidation of sarcosine and N-alkyl derivatives of  
glycine by D-amino-acid oxidase

AUTHOR(S): Naoi, Makoto; Yagi, Kunio

CORPORATE SOURCE: Fac. Med., Univ. Nagoya, Nagoya, Japan  
SOURCE: Biochimica et Biophysica Acta (1976),  
438(1), 61-70  
CODEN: BBACAQ; ISSN: 0006-3002  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
IT 627-01-0 3182-81-8 25303-14-4  
35386-27-7 41331-10-6  
RL: BIOL (Biological study)  
(amino acid oxidase specificity for)  
RN 627-01-0 HCAPLUS  
CN Glycine, N-ethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

EtNH-CH<sub>2</sub>-CO<sub>2</sub>H

RN 3182-81-8 HCAPLUS  
CN Glycine, N-butyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

n-BuNH-CH<sub>2</sub>-CO<sub>2</sub>H

RN 25303-14-4 HCAPLUS  
CN Glycine, N-propyl- (6CI, 8CI, 9CI) (CA INDEX NAME)

n-PrNH-CH<sub>2</sub>-CO<sub>2</sub>H

RN 35386-27-7 HCAPLUS  
CN Glycine, N-pentyl- (6CI, 9CI) (CA INDEX NAME)

Me-(CH<sub>2</sub>)<sub>4</sub>-NH-CH<sub>2</sub>-CO<sub>2</sub>H

RN 41331-10-6 HCAPLUS  
CN Glycine, N-hexyl- (9CI) (CA INDEX NAME)

Me-(CH<sub>2</sub>)<sub>5</sub>-NH-CH<sub>2</sub>-CO<sub>2</sub>H

AB Sarcosine was oxidized by D-amino acid oxidase (EC 1.4.3.3) to yield methylamine and glyoxylic acid. A series of N-alkyl glycines were also oxidized by this enzyme. N-acetyl- and N-phenylglycine inhibited the oxidase by competing with the substrate, whereas N-methyl-N-acetylglycine did not bind to the enzyme. This suggests the requirement of at least 1 unsubstituted H atom at the amino group of glycine for binding. The primary step in the reaction was the release of a proton from the substrate, indicating the formation of a substituted imino acid, which was spontaneously hydrolyzed to glyoxylic acid and an amine.

L38 ANSWER 21 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 1975:514857 HCAPLUS  
DOCUMENT NUMBER: 83:114857  
TITLE: Preparation of N-alkyl and N-arylglycines from  
glyoxylic acid using carbonylhydridoferrate as a



reducing agent  
 AUTHOR(S): Watanabe, Yoshihisa; Shim, Sang Chul; Mitsudo, Takeaki; Yamashita, Masakazu; Takegami, Yoshinobu  
 CORPORATE SOURCE: Fac. Eng., Kyoto Univ., Kyoto, Japan  
 SOURCE: Chemistry Letters (1975), (7), 699-700  
 CODEN: CMLTAG; ISSN: 0366-7022  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 IT 3182-82-9P 56676-69-8P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 3182-82-9 HCAPLUS  
 CN Glycine, N-butyl-, hydrochloride (7CI, 8CI, 9CI) (CA INDEX NAME)

n-BuNH-CH<sub>2</sub>-CO<sub>2</sub>H

● HCl

RN 56676-69-8 HCAPLUS  
 CN Glycine, N-hexyl-, hydrochloride (9CI) (CA INDEX NAME)

Me-(CH<sub>2</sub>)<sub>5</sub>-NH-CH<sub>2</sub>-CO<sub>2</sub>H

● HCl

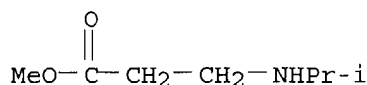
AB To Fe(CO)<sub>5</sub> and alc. in KOH was added an amine, glyoxylic acid and EtOH and the mixture stirred 24 hr at room temperature The precipitate was acidified with concentrate  
 HCl to give salts of glycines, RNHCH<sub>2</sub>CO<sub>2</sub>H·HCl (R = Me, Bu, hexyl, cyclohexyl, PhCH<sub>2</sub>, Ph, p-MeC<sub>6</sub>H<sub>4</sub>, p-MeOC<sub>6</sub>H<sub>4</sub>, p-ClC<sub>6</sub>H<sub>4</sub>, β-naphthyl.

L38 ANSWER 22 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1975:409540 HCAPLUS  
 DOCUMENT NUMBER: 83:9540  
 TITLE: Alkyl 5-oxoalkanoates  
 INVENTOR(S): Mueller, Werner  
 PATENT ASSIGNEE(S): Farbwerke Hoechst A.-G.  
 SOURCE: Ger. Offen., 11 pp.  
 CODEN: GWXXBX  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

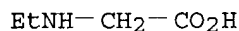
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2325160	A1	19741205	DE 1973-2325160	19730518 <--
ZA 7402951	A	19750528	ZA 1974-2951	19740508 <--
IN 141915	A	19770430	IN 1974-CA1033	19740509 <--
NL 7406400	A	19741120	NL 1974-6400	19740513 <--
CH 593902	A	19771230	CH 1974-6689	19740515 <--
IT 1012464	A	19770310	IT 1974-22850	19740516 <--

FR 2229679 A1 19741213 FR 1974-17272 19740517 <--  
 FR 2229679 B1 19781117  
 JP 50030829 A2 19750327 JP 1974-54612 19740517 <--  
 BE 815282 A1 19741120 BE 1974-144528 19740520 <--  
 GB 1473184 A 19770511 GB 1974-22412 19740520 <--  
 PRIORITY APPLN. INFO.: DE 1973-2325160 19730518 <--  
 IT 42313-51-9  
 RL: CAT (Catalyst use); **USES (Uses)**  
 (catalyst, for ketone addition to alkyl acrylates)  
 RN 42313-51-9 HCAPLUS  
 CN  $\beta$ -Alanine, N-(1-methylethyl)-, methyl ester (9CI) (CA INDEX NAME)

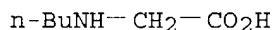


AB Fifteen RCOCHR1CH2CHR2CO2R3 [R = Me, Et, Bu, or Ph; R1 = H, Me, Pr, or Ph; or RR1 = (CH2)4; R2 = H or Me; R3 = C1-4 alkyl] or their mixts. were prepared by reaction of RCOCH2R1 with CH2:CR2CO2R3 in the presence of amines. Thus, Me2CO and CH2:CHCO2Me were autoclaved in the presence of aqueous Me2CHNH2 and BzOH at 180° to give 84.5% MeCO(CH2)3CO2Me and < 10% (MeO2CCH2CH2)2CHCOMe.

L38 ANSWER 23 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN  
 ACCESSION NUMBER: 1974:888 HCAPLUS  
 DOCUMENT NUMBER: 80:888  
 TITLE: Diffusion of glycine and N-substituted glycines across bimolecular lipid membranes  
 AUTHOR(S): Stillwell, William; Winter, Harry C.  
 CORPORATE SOURCE: Dep. Biochem., Pennsylvania State Univ., University Park, PA, USA  
 SOURCE: Biochemical and Biophysical Research Communications (1973), 54(4), 1437-43  
 CODEN: BBRCA9; ISSN: 0006-291X  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 IT 627-01-0 3182-81-8 41331-10-6  
 50997-13-2  
 RL: PEP (Physical, engineering or chemical process); PROC (Process) (diffusion of, across liposome)  
 RN 627-01-0 HCAPLUS  
 CN Glycine, N-ethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RN 3182-81-8 HCAPLUS  
 CN Glycine, N-butyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RN 41331-10-6 HCAPLUS  
 CN Glycine, N-hexyl- (9CI) (CA INDEX NAME)

Me- (CH<sub>2</sub>)<sub>5</sub>-NH-CH<sub>2</sub>-CO<sub>2</sub>H

RN 50997-13-2 HCAPLUS  
CN Glycine, N-nonyl- (9CI) (CA INDEX NAME)

Me- (CH<sub>2</sub>)<sub>8</sub>-NH-CH<sub>2</sub>-CO<sub>2</sub>H

AB Free glycine diffused very slowly across synthetic bimol. lipid membranes, whereas several N-substituted derivs. of glycine penetrated the membranes more readily. Pyridoxal, formaldehyde, and acetaldehyde enhanced the diffusion of glycine across the membranes, presumably the result of imine formation between the aldehyde and the  $\alpha$ -amino group of glycine. Several N-substituted glycines were synthesized and their rates of efflux from liposomes were related to their H<sub>2</sub>O-CHCl<sub>3</sub> partition coeffs. This is the 1st demonstration of carrier-mediated diffusion of amino acids across a bimol. lipid membrane.

L38 ANSWER 24 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1973:101277 HCAPLUS

DOCUMENT NUMBER: 78:101277

TITLE: Synergistic combinations for inhibiting the attack of alkaline solutions on alkali-sensitive substrates

INVENTOR(S): Dupre, Jean; Booman, Keith A.

PATENT ASSIGNEE(S): Rohm and Haas Co.

SOURCE: U.S., 7 pp.

CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3653095	A	19720404	US 1969-835906	19690618 <--
GB 1320793	A	19730620	GB 1970-29430	19700617 <--
PRIORITY APPLN. INFO.:			US 1969-834499	19690618 <--
			US 1969-835906	19690618 <--

IT 1462-54-0 41331-10-6 41331-11-7

RL: USES (Uses)

(corrosion inhibition by, of alkaline solns.)

RN 1462-54-0 HCAPLUS

CN  $\beta$ -Alanine, N-dodecyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

Me- (CH<sub>2</sub>)<sub>11</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-CO<sub>2</sub>H

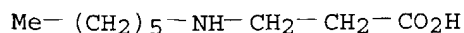
RN 41331-10-6 HCAPLUS

CN Glycine, N-hexyl- (9CI) (CA INDEX NAME)

Me- (CH<sub>2</sub>)<sub>5</sub>-NH-CH<sub>2</sub>-CO<sub>2</sub>H

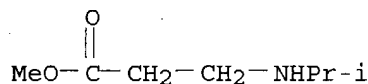
RN 41331-11-7 HCAPLUS

CN  $\beta$ -Alanine, N-hexyl- (9CI) (CA INDEX NAME)



AB During cleaning with an aqueous alkaline solution containing 0.1-10 weight % alkali, materials (e.g. Al, Zn, Sn, Pb, their alloys, Si oxides and compds. containing Si oxides) which are sensitive to the alkaline attack are protected by a synergistic combination of:  $\geq 1$  metal ion (0.005M) such as  $\text{Ba}^{2+}$ ,  $\text{Ca}^{2+}$ , and  $\text{Sr}^{2+}$  with  $\geq 1$  surface-active agent (0.5 weight %) selected from alkyl glycosides having a formula  $\text{ROGmH}$ , where G is a glycosyl radical, R is  $\text{C}_6$ -16 alkyl connected to C-1 of the glycosyl radical through the O, and  $m = 1-4$ ; or ethylene oxide adducts of the alkyl glycosides containing  $\leq 2$  ethylene oxide units per glycosyl radical; or amino carboxylic acids having  $\text{C} \geq 10$  and metal salts of amino carboxylic acids (0.01-5 weight %). Optionally in certain and essentially in other applications, a  $\text{H}_2\text{O}$ -soluble naphthalene derivative may be added to the synergistic combination.

L38 ANSWER 25 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN  
 ACCESSION NUMBER: 1973:38037 HCAPLUS  
 DOCUMENT NUMBER: 78:38037  
 TITLE: Potential hypotensive compounds. Substituted 3-aminopropionates and 3-aminopropionohydroxamic acids  
 AUTHOR(S): Biggs, D. F.; Coutts, R. T.; Selley, M. L.; Towill, G. A.  
 CORPORATE SOURCE: Fac. Pharm. Pharm. Sci., Univ. Alberta, Edmonton, AB, Can.  
 SOURCE: Journal of Pharmaceutical Sciences (1972), 61(11), 1739-45  
 CODEN: JPMSAE; ISSN: 0022-3549  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 IT 40870-77-7P  
 RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and hypotensive effect of)  
 RN 40870-77-7 HCAPLUS  
 CN  $\beta$ -Alanine, N-(1-methylethyl)-, methyl ester, hydrochloride (9CI) (CA INDEX NAME)



● HCl

AB Most of the 48 3-aminopropionate esters studied were synthesized by addition of an amine across the  $\alpha,\beta$ -double bond of Me acrylate [96-33-3], Me methacrylate [80-62-6], or Me crotonate [18707-60-3], while the remainder were obtained by interaction of 1 mole of a 3-bromopropionic ester with 2 moles of the corresponding amine. Twenty-six 3-aminopropionohydroxamic acid hydrochlorides were prepared by treatment of the appropriate amino ester with hydroxylamine-HCl [5470-11-1] in MeOH. Many of the compds. such as 2-methyl-3-[(2-phenylethyl)amino]propanoic acid Me ester [6297-67-2], 3,3'-[(2-phenylethyl)imino]bispropanoic acid dimethyl ester [38129-46-3], N-[3-(hydroxyamino)-2-methyl-3-

oxopropyl]heptanaminium chloride [38129-47-4], and N-[3-(hydroxyamino)-3-oxopropyl]-2-(2-phenylethyl)benzeneethanaminium chloride [38202-84-5] possessed hypotensive properties but of very short duration. 2-Methyl-3-(octylamino)propanoic acid Me ester [29228-46-4] was the most active, and at 4 mg/kg i.v. decreased the blood pressure of rats by an average of 52% for 12 min. Some of the compds. were screened for their ability to protect mice against a lethal dose of diisopropylfluorophosphate [55-91-4], but none was active.

L38 ANSWER 26 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN  
 ACCESSION NUMBER: 1971:75986 HCAPLUS  
 DOCUMENT NUMBER: 74:75986  
 TITLE: Synthesis and properties of some hypotensive  
 N-alkylaminopropionic esters and N,N-  
 dialkylaminopropionic esters and their hydroxamic  
 acids  
 AUTHOR(S): Coutts, Ronald T.; Hubbard, J. W.; Midha, Kamal K.;  
 Prasad, Kailash  
 CORPORATE SOURCE: Fac. Pharm. Pharm. Sci., Univ. Alberta, Edmonton, AB,  
 Can.  
 SOURCE: Journal of Pharmaceutical Sciences (1971),  
 60(1), 28-33  
 CODEN: JPMSAE; ISSN: 0022-3549  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 IT 10478-41-8P 31044-47-0P 31044-48-1P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 10478-41-8 HCAPLUS  
 CN  $\beta$ -Alanine, N-ethyl- (7CI, 8CI, 9CI) (CA INDEX NAME)

EtNH-CH<sub>2</sub>-CH<sub>2</sub>-CO<sub>2</sub>H

RN 31044-47-0 HCAPLUS  
 CN  $\beta$ -Alanine, N-hexyl-, methyl ester (8CI, 9CI) (CA INDEX NAME)

$$\text{MeO}-\overset{\text{O}}{\parallel}{\text{C}}-\text{CH}_2-\text{CH}_2-\text{NH}-(\text{CH}_2)_5-\text{Me}$$

RN 31044-48-1 HCAPLUS  
 CN  $\beta$ -Alanine, N-hexyl-, methyl ester, hydrochloride (8CI, 9CI) (CA INDEX NAME)

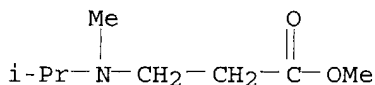
$$\text{MeO}-\overset{\text{O}}{\parallel}{\text{C}}-\text{CH}_2-\text{CH}_2-\text{NH}-(\text{CH}_2)_5-\text{Me}$$

● HCl

GI For diagram(s), see printed CA Issue.  
 AB Thirty-eight 3-(N-alkylamino)- and 3-(N,N-dialkylamino)propionic esters

(I), hydroxamic acids (II), carboxylic acids, and related compds. were synthesized and the majority of the esters and hydroxamic acids decreased the blood pressure of anesthetized cats, while the carboxylic acids were inactive. The esters were prepared by the interaction of methyl acrylate or methyl methacrylate and an appropriate amine. Some hindered amines did not react with the acrylate, and some esters hydrolyzed to the corresponding carboxylic acids when stored even for a short time. The hydroxamic acids were prepared from the amino esters treated with hydroxylamine.

L38 ANSWER 27 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN  
 ACCESSION NUMBER: 1970:445265 HCAPLUS  
 DOCUMENT NUMBER: 73:45265  
 TITLE: Derivatives of substituted acetic acids. XXVIII.  
 Dialkylaminopropyl esters of  $\alpha$ -  
 naphthylheterylacetic acids  
 AUTHOR(S): Mndzhoyan, A. L.; Badalyan, V. E.  
 CORPORATE SOURCE: Inst. Tonkoi Org. Khim., Erevan, USSR  
 SOURCE: Armyanskii Khimicheskii Zhurnal (1970),  
 23(4), 258-67  
 CODEN: AYKZAN; ISSN: 0515-9628  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Russian  
 IT 27453-30-1P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 27453-30-1 HCAPLUS  
 CN  $\beta$ -Alanine, N-methyl-N-(1-methylethyl)-, methyl ester (9CI) (CA INDEX  
 NAME)



AB A mixture of 0.5 mole  $\text{R}_1\text{R}_2\text{NH}$ , 0.5 mole  $\text{CH}_2:\text{CHCO}_2\text{Me}$ , in 200 ml  $\text{C}_6\text{H}_6$  refluxed for 6-8 hr (with  $\text{iso-PrR}_2\text{NH}$ , the mixture was heated at  $95^\circ$  in a sealed tube 16-20 hr while with  $(\text{iso-Pr})_2\text{NH}$  similarly treated for 150 hr, to give  $\text{R}_1\text{R}_2\text{NCH}_2\text{CH}_2\text{CO}_2\text{Me}$  (I).  $\text{LiAlH}_4$  reduction of (I) gave  $\text{R}_1\text{R}_2\text{NCH}_2\text{CH}_2\text{CH}_2\text{OH}$  (II) which, in refluxing  $\text{PhMe}$ , reacted with  $\alpha\text{-C}_{10}\text{H}_7\text{CHClCOCl}$  (III) [from  $\alpha\text{-C}_{10}\text{H}_7\text{CH}(\text{OH})\text{CO}_2\text{H}$  (50.5 g) and refluxing  $\text{SOCl}_2$  (180 ml)] to give the corresponding  $\alpha\text{-C}_{10}\text{H}_7\text{CHClCO}_2(\text{CH}_2)_3\text{NR}_1\text{R}_2$  (IV). IV treated with an amine yielded the title  $\alpha\text{-C}_{10}\text{H}_7\text{CHR}_3\text{CO}_2(\text{CH}_2)_3\text{NR}_1\text{R}_2$  (V). Thus a mixture of 0.025 mole IV, 0.05 mole piperidine, and 100 ml  $\text{PhMe}$  refluxed 6-8 hr gave 77% V ( $\text{R}_1 = \text{R}_2 = \text{Me}$ ,  $\text{R}_3 = \text{piperidino}$ ), b<sub>3</sub> 228-30°. The morpholino analog was similarly prepared. Approx. 150 new compds. and derivs. were reported.

L38 ANSWER 28 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN  
 ACCESSION NUMBER: 1967:517255 HCAPLUS  
 DOCUMENT NUMBER: 67:117255  
 TITLE: Preparation of N-substituted aspartic esters,  
 $\beta$ -amino esters, and their corresponding acids  
 AUTHOR(S): Pfau, Michel  
 CORPORATE SOURCE: Lab. Chim. Ecole Norm. Super., Paris, Fr.  
 SOURCE: Bulletin de la Societe Chimique de France (  
 1967), (4), 1117-25  
 CODEN: BSCFAS; ISSN: 0037-8968  
 DOCUMENT TYPE: Journal

LANGUAGE: French  
OTHER SOURCE(S): CASREACT 67:117255  
IT 16217-35-9P 16270-07-8P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation and N.M.R. of)  
RN 16217-35-9 HCAPLUS  
CN  $\beta$ -Alanine, N-(1-methylethyl)- (9CI) (CA INDEX NAME)

i-PrNH-CH<sub>2</sub>-CH<sub>2</sub>-CO<sub>2</sub>H

RN 16270-07-8 HCAPLUS  
CN  $\beta$ -Alanine, N-propyl- (8CI, 9CI) (CA INDEX NAME)

n-PrNH-CH<sub>2</sub>-CH<sub>2</sub>-CO<sub>2</sub>H

AB Et acrylate (I), diethyl fumarate (II), dimethyl maleate (III), MeCH:CHCO<sub>2</sub>Et (IV), and CH<sub>2</sub>:CMeCO<sub>2</sub>Me (V) are treated with PrNH<sub>2</sub>, iso-PrNH<sub>2</sub>, and Et<sub>2</sub>NH to give amino acids. Thus, a mixture of 0.05 mole I and 0.5 mole PrNH<sub>2</sub> is kept 24 hrs. to give Et  $\beta$ -propylaminopropionate, b0.1 32°. A mixture of 5.0 g. I and 1.5 g. PrNH<sub>2</sub> is refluxed 10 hrs. to give diethyl  $\beta$ , $\beta'$ -propyliminodipropionate, b0.4 98°. Also prepared are (reactants, product, b.p./mm., and m.p. given): iso-PrNH<sub>2</sub> and I, iso-PrNHCH<sub>2</sub>CH<sub>2</sub>CO<sub>2</sub>Et, 38°/0.4, -; iso-PrNH<sub>2</sub> and I, iso-PrN(CH<sub>2</sub>CH<sub>2</sub>CO<sub>2</sub>Et)<sub>2</sub>, 92°/0.05, -; Et<sub>2</sub>NH and I, Et<sub>2</sub>NCH<sub>2</sub>CH<sub>2</sub>CO<sub>2</sub>Et, 28°/0.08, -; PrNH<sub>2</sub> and IV, MeCH(NHPr)CH<sub>2</sub>CO<sub>2</sub>Et, 36°/0.15, -; iso-PrNH<sub>2</sub> and IV, Me(iso-PrNH)CHCH<sub>2</sub>CO<sub>2</sub>Et, 77°/11, -; PrNH<sub>2</sub> and V, PrNHCH<sub>2</sub>CHMeCO<sub>2</sub>Me, 31°/0.15, -; iso-PrNH<sub>2</sub> and V, iso-PrNHCH<sub>2</sub>CHMeCO<sub>2</sub>Me, 41°/0.1, -; PrNH<sub>2</sub> and III, MeO<sub>2</sub>CCH<sub>2</sub>CH(NHPr)CO<sub>2</sub>Me, 65-6°/0.15, -; iso-PrNH<sub>2</sub> and III, MeO<sub>2</sub>CCH<sub>2</sub>CH(NHPr-iso)CO<sub>2</sub>Me, 70°/0.3, -; Et<sub>2</sub>NH and III, MeO<sub>2</sub>CCH(NEt<sub>2</sub>)CH<sub>2</sub>CO<sub>2</sub>Me, 64°/0.3, -; PrNH<sub>2</sub> and II, EtO<sub>2</sub>CCH(NHPr)CH<sub>2</sub>CO<sub>2</sub>Et, 91°/0.3, -; iso-PrNH<sub>2</sub> and II, EtO<sub>2</sub>CCH(NHPr-iso)CH<sub>2</sub>CO<sub>2</sub>Et, 84°/0.4, -; Et<sub>2</sub>NH and II, EtO<sub>2</sub>CCH(NEt<sub>2</sub>)CH<sub>2</sub>CO<sub>2</sub>Et, 62°/0.1, -; piperidine and III, di-Me N,N-pentamethyleneaspartate, 98-101°/0.5, 44-4.5°; piperidine and III, Me  $\alpha$ -piperidino- $\beta$ -piperidinocarbonylpropionate, -, 182-3° (decomposition). Also prepared are iso-PrNHCHMeCH<sub>2</sub>CO<sub>2</sub>Et-HCl, m. 118.5-19.5°, and iso-PrNHCH<sub>2</sub>CHMeCO<sub>2</sub>Me.HCl, m. 114-14.5°. The esters are hydrolyzed to give the following acids (m.p. given): PrNHCH<sub>2</sub>CH<sub>2</sub>CO<sub>2</sub>H, 150.5-1.5°; iso-PrNHCH<sub>2</sub>CH<sub>2</sub>CO<sub>2</sub>H, 165-6°; Et<sub>2</sub>NCH<sub>2</sub>CH<sub>2</sub>CO<sub>2</sub>H, 68-70°; Me(PrNH)CHCH<sub>2</sub>CO<sub>2</sub>H, 142-3°; Me(iso-PrNH)CHCH<sub>2</sub>CO<sub>2</sub>H, 165-6°; PrNHCH<sub>2</sub>CHMeCO<sub>2</sub>H, 136-7°; iso-PrNHCH<sub>2</sub>CHMeCO<sub>2</sub>H, 170.5-1.0°; MeO<sub>2</sub>C(PrNH)CHCH<sub>2</sub>CO<sub>2</sub>H, 151°; MeO<sub>2</sub>C(iso-PrNH)CHCH<sub>2</sub>CO<sub>2</sub>H, 120.5-21°; EtO<sub>2</sub>C(PrNH)CHCH<sub>2</sub>CO<sub>2</sub>H, 165-7°; EtO<sub>2</sub>C(iso-PrNH)CHCH<sub>2</sub>CO<sub>2</sub>H, 94-5°, HO<sub>2</sub>CCH(NHPr-iso)CH<sub>2</sub>CO<sub>2</sub>H, 170-2°. N.M.R. data are given for the prepared compds.

L38 ANSWER 29 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 1966:451518 HCAPLUS  
DOCUMENT NUMBER: 65:51518  
ORIGINAL REFERENCE NO.: 65:9660g-h,9661a  
TITLE: Systemic fungicides  
INVENTOR(S): Harnack, Willy; Schwarz, Justus  
SOURCE: 3 pp.  
DOCUMENT TYPE: Patent

LANGUAGE: Unavailable

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	DD 45884		19660205	DD	19641224 <--
	GB 1048507			GB	
IT	542-53-0, Glycine, N-ethyl-, hydrochloride		627-01-0,		
	Glycine, N-ethyl- 3182-82-9, Glycine, N-butyl-, hydrochloride				
	3182-86-3, Glycine, N-isobutyl-, hydrochloride		3183-23-1		
	, Glycine, N-isopropyl-, ethyl ester, hydrochloride		3338-22-5,		
	Glycine, N-isopropyl-, hydrochloride		6939-13-5, Glycine,		
	N-propyl-, hydrochloride				
	(as fungicide)				
RN	542-53-0	HCAPLUS			
CN	Glycine, N-ethyl-, hydrochloride	(7CI, 8CI, 9CI)	(CA INDEX NAME)		

 $\text{EtNH}-\text{CH}_2-\text{CO}_2\text{H}$ 

● HCl

RN 627-01-0 HCAPLUS  
CN Glycine, N-ethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

 $\text{EtNH}-\text{CH}_2-\text{CO}_2\text{H}$ 

RN 3182-82-9 HCAPLUS  
CN Glycine, N-butyl-, hydrochloride (7CI, 8CI, 9CI) (CA INDEX NAME)

 $\text{n-BuNH}-\text{CH}_2-\text{CO}_2\text{H}$ 

● HCl

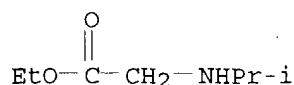
RN 3182-86-3 HCAPLUS  
CN Glycine, N-(2-methylpropyl)-, hydrochloride (9CI) (CA INDEX NAME)

 $\text{i-BuNH}-\text{CH}_2-\text{CO}_2\text{H}$ 

● HCl

RN 3183-23-1 HCAPLUS  
CN Glycine, N-(1-methylethyl)-, ethyl ester, hydrochloride (9CI) (CA INDEX NAME)

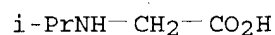




● HCl

RN 3338-22-5 HCAPLUS

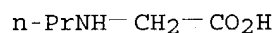
CN Glycine, N-(1-methylethyl)-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 6939-13-5 HCAPLUS

CN Glycine, N-propyl-, hydrochloride (7CI, 8CI, 9CI) (CA INDEX NAME)



● HCl

AB Glycine derivs. of the general formula  $\text{RHNCH}_2\text{CO}_2\text{R}'$  ( $\text{R} = \text{H}, \text{Me}, \text{or Et}$ ) were systemic fungicides in vivo but not in vitro (spore germination test). Four young tomato plants with 4 or 5 leaves, in plastic pots were treated 2 times at 2-day intervals at the root stock with 3 ml. of test solution. Two days later they were sprayed with a spore suspension of *Phytophthora infestans*, then placed in a moist chamber. After 4 days each plant was scored for fungus infestation on scale 0, 1, 2, 3, or 4 meaning no, mild, median, marked infestation, or plant destroyed, resp. Scores for water alone and for each fungicide in replicate rests were summed. The sum for water was set at 100, and the relative scores of fungicides recorded. For 8 plants so treated with N-ethylglycine (I), N-ethylglycine-HCl (II), N-propylglycine-HCl (III), and N-2-hydroxyethylglycine (IV) in 0.5% solns., the relative infection scores were 0, 6, 10, 11, resp., and for 0.25% solns. 12, 10, 25, 20, resp. Eight plants sprayed sop. with solns. of II, III, and N-isopropylglycine-HCl were protected to a similar extent. Celery plants were protected against *Septoria apii* by root stock immersion in 0.5 and 0.25% solns. of the methyl esters and the methyl ester hydrochlorides of N-isopropylglycine and N-allylglycine, the Et ester of N-allylglycine, and N-butylglycine, N-isobutylglycine hydrochlorides. Areas of infection were usually smaller than in the controls. Development of reproductive structures is practically completely depressed.

L38 ANSWER 30 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1965:480952 HCAPLUS

DOCUMENT NUMBER: 63:80952

ORIGINAL REFERENCE NO.: 63:14970h,14971a-b

TITLE: Monoalkylated glycine derivatives

AUTHOR(S): Hanke, H.

CORPORATE SOURCE: Univ. Jena, GA

SOURCE: Pharmazeutische Zentralhalle fuer Deutschland (1960), 99(June), 318-22  
From: CZ 1963(26), 10820-1.  
CODEN: PHZEAD; ISSN: 0369-9773

DOCUMENT TYPE: Journal  
LANGUAGE: German

IT 542-53-0, Glycine, N-ethyl-, hydrochloride 627-01-0,  
Glycine, N-ethyl- 3182-81-8, Glycine, N-butyl- 3182-82-9  
, Glycine, N-butyl-, hydrochloride 3182-85-2, Glycine,  
N-isobutyl- 3182-86-3, Glycine, N-isobutyl-, hydrochloride  
3182-89-6, Glycine, N-isohexyl- 3182-90-9, Glycine,  
N-isohexyl-, hydrochloride 3183-21-9, Glycine, N-isopropyl-  
3183-22-0, Glycine, N-isopropyl-, ethyl ester 3183-23-1,  
Glycine, N-isopropyl-, ethyl ester, hydrochloride 3338-22-5,  
Glycine, N-isopropyl-, hydrochloride  
(preparation of)

RN 542-53-0 HCAPLUS  
CN Glycine, N-ethyl-, hydrochloride (7CI, 8CI, 9CI) (CA INDEX NAME)

EtNH-CH<sub>2</sub>-CO<sub>2</sub>H

● HCl

RN 627-01-0 HCAPLUS  
CN Glycine, N-ethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

EtNH-CH<sub>2</sub>-CO<sub>2</sub>H

RN 3182-81-8 HCAPLUS  
CN Glycine, N-butyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

n-BuNH-CH<sub>2</sub>-CO<sub>2</sub>H

RN 3182-82-9 HCAPLUS  
CN Glycine, N-butyl-, hydrochloride (7CI, 8CI, 9CI) (CA INDEX NAME)

n-BuNH-CH<sub>2</sub>-CO<sub>2</sub>H

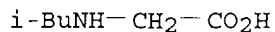
● HCl

RN 3182-85-2 HCAPLUS  
CN Glycine, N-(2-methylpropyl)- (9CI) (CA INDEX NAME)

i-BuNH-CH<sub>2</sub>-CO<sub>2</sub>H

RN 3182-86-3 HCAPLUS

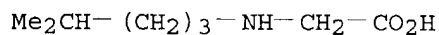
CN Glycine, N-(2-methylpropyl)-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

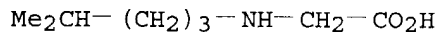
RN 3182-89-6 HCAPLUS

CN Glycine, N-isohexyl- (7CI, 8CI) (CA INDEX NAME)



RN 3182-90-9 HCAPLUS

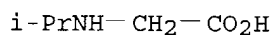
CN Glycine, N-isohexyl-, hydrochloride (7CI, 8CI) (CA INDEX NAME)



● HCl

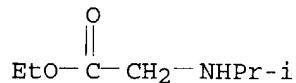
RN 3183-21-9 HCAPLUS

CN Glycine, N-(1-methylethyl)- (9CI) (CA INDEX NAME)



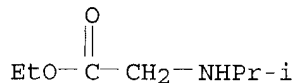
RN 3183-22-0 HCAPLUS

CN Glycine, N-(1-methylethyl)-, ethyl ester (9CI) (CA INDEX NAME)



RN 3183-23-1 HCAPLUS

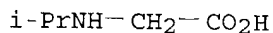
CN Glycine, N-(1-methylethyl)-, ethyl ester, hydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 3338-22-5 HCAPLUS

CN Glycine, N-(1-methylethyl)-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

AB Primary amine HCl salts with HCHO and KCN yield alkylamino-acetonitriles which can be hydrolyzed with alc. HCl to N-alkylglycines Et ester HCl salts. These treated with  $\text{NH}_3\text{-CHCl}_3$  yield the free esters which are converted by acid saponification to the alkylglycine (Ia) and their HCl salts. Thus, to obtain N-ethylglycine (I), m. 180-2° (decomposition), I.HCl is treated with AgOH in water, the mixture filtered, the filtrate gassed with  $\text{H}_2\text{S}$ , filtered, concentrated, and the residue dissolved in EtOH-Et<sub>2</sub>O. I.HCl m. 179-80°, is prepared by boiling 3 hrs. the Et ester (II) in 6N HCl, evaporating, and dissolving in EtOH-Et<sub>2</sub>O. To prepare II.HCl, m. 135°, HCHO, EtNH<sub>2</sub>.HCl, and KCN are allowed to react 30 min. in aqueous solution at 5° under CO<sub>2</sub>, the mixture kept several hrs., the nitrile formed extracted with Et<sub>2</sub>O (yield 90-100%), boiled 4 hrs. with ethanolic HCl, the NH<sub>4</sub>Cl filtered off and the filtrate concentrated; yield 90-100%. II, b<sub>16</sub> 58°, is obtained by 30-min. reaction of II.HCl and  $\text{NH}_3\text{-CHCl}_3$  at 0° filtering and distilling; yield 55-75%. Similarly were prepared the following Ia (alkyl, m.p., m.p. HCl salt, b.p. Et ester, and m.p. Et ester HCl salt given): isopropyl, 193-5° (decomposition), 202-3°, b<sub>2-3</sub> 32-5°, 113-15° (decomposition); allyl, 158-9° (decomposition), 167-9° (decomposition), b<sub>3</sub> 47°, 113-14° (decomposition) (EtOH); n-butyl, 190-1° (decomposition), 202-4°, b<sub>2-3</sub> 47-51°, 164-6°; isobutyl, 192-3° (decomposition), 210-12° (decomposition) or 221-222° (in sealed tube), b<sub>3</sub> 49-51°, 127-8.5° (decomposition); isohexyl, 194-5°, 186-7° b<sub>4</sub> 79°, 182-3°.

L38 ANSWER 31 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1963:435 HCAPLUS

DOCUMENT NUMBER: 58:435

ORIGINAL REFERENCE NO.: 58:63e

TITLE: Physicochemical analysis of isopropylamine-ethyl monochloroacetate system

AUTHOR(S): Bekturov, E. A.

SOURCE: Izvestiya Akademii Nauk Kazakhskoi SSR, Seriya Khimicheskaya (1962), (1), 44-8  
CODEN: IKAKAK; ISSN: 0002-3205

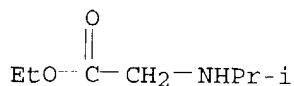
DOCUMENT TYPE: Journal

LANGUAGE: Russian

IT 3183-22-0, Glycine, N-isopropyl-, ethyl ester 3183-23-1, Glycine, N-isopropyl-, ethyl ester, hydrochloride (formation of)

RN 3183-22-0 HCAPLUS

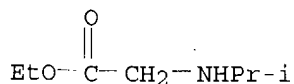
CN Glycine, N-(1-methylethyl)-, ethyl ester (9CI) (CA INDEX NAME)



RN 3183-23-1 HCAPLUS

CN Glycine, N-(1-methylethyl)-, ethyl ester, hydrochloride (9CI) (CA INDEX

NAME)



● HCl

AB Measurement of viscosity, d., and conductivity of system  $\text{Me}_2\text{CHNH}_2 + \text{CH}_2\text{-ClCO}_2\text{Et}$  shows the formation of  $(\text{Me}_2\text{CHNH}_2\text{CH}_2\text{CO}_2\text{Et})^+ \cdot \text{Cl}^-$ , which then reacts with the 2nd mol. of amine to form  $\text{Me}_2\text{CHNHCH}_2\text{CO}_2\text{Et}$  and  $\text{Me}_2\text{CHNH}_3\text{Cl}$ .

L38 ANSWER 32 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1956:52502 HCAPLUS

DOCUMENT NUMBER: 50:52502

ORIGINAL REFERENCE NO.: 50:10024h-i,10025a-d

TITLE: The preparation of substituted hydrazines. III. A general method for preparing N-substituted glycines

AUTHOR(S): Tien, Jack M.; Hunsberger, I. Moyer

CORPORATE SOURCE: Antioch Coll., Yellow Springs, O.

SOURCE: Journal of the American Chemical Society (1955), 77, 6696-8

CODEN: JACSAT; ISSN: 0002-7863

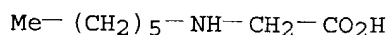
DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

IT 56676-69-8, Glycine, N-hexyl-, hydrochloride (preparation of)

RN 56676-69-8 HCAPLUS

CN Glycine, N-hexyl-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

AB cf. C.A. 50, 3431c.  $\text{C}_6\text{H}_{13}\text{NH}_2$  (0.765 g.) and 1.7 g.  $\text{HOCH}_2\text{CO}_2\text{Et}$  (62% pure) in 10 cc. glacial AcOH allowed to stand 2 hrs., hydrogenated with shaking 2 hrs. at room temperature and 3-4 atmospheric pressure over 0.1 g. 10% Pd-C, the colorless filtrate neutralized with solid  $\text{NaHCO}_3$  and extracted with two 60-cc. portions Et<sub>2</sub>O, the residue from the extract refluxed 10 min. with 5 cc. 10% aqueous NaOH, cooled, and acidified with 2-3 cc. concentrated HCl, and the precipitated small, nearly white plates, m. 200-6°, heated with 25 cc. glacial AcOH on a steam bath, filtered hot, and cooled gave 0.4 g. N-hexylglycine (I) HCl salt, white flakes, m. 215-18°. The filtrate from the hydrogenation basified with dilute aqueous NaOH, refluxed cooled, acidified with excess concentrated HCl, and evaporated to dryness, and the residue extracted with hot glacial AcOH gave I.HCl.  $\text{C}_6\text{H}_{13}\text{NH}_2$  and  $\text{HOCH}_2\text{CO}_2\text{Et}$  in 2:3 concentrated HCl-H<sub>2</sub>O gave only a very low yield of I.HCl; no I.HCl was detected from a hydrogenation in 6N HCl.  $\text{PhNH}_2$  (1.00 g.) in 5 cc. 95% EtOH and 1.70 g.

HOCH<sub>2</sub>CO<sub>2</sub>Et (62% pure) hydrogenated 2.5 hrs. and filtered, the catalyst washed with 10 cc. 95% EtOH, and the combined filtrate and washings diluted to the cloud point with H<sub>2</sub>O and cooled gave 1.06 g. N-phenylglycine Et ester (II), white plates, m. 57-8°; 2nd and 3rd crops, 0.41 and 0.17 g., resp. II (0.179 g.) refluxed 10 min. with 2 cc. concentrated HCl and

4

cc. H<sub>2</sub>O and evaporated to dryness in vacuo, the white residue dissolved with warming with 2 cc. concentrated HCl on the steam bath, and the solution cooled gave

0.116 g. N-phenylglycine-HCl salt, m. 172-4°; 2nd crop, 0.041 g. Com. N-phenylglycine (0.1 g.), yellow powder, and 0.1 g. NaCl dissolved at about 70° in 5 cc. H<sub>2</sub>O, and the solution cooled deposited after about 2 min. large pale-yellow needles; a similar recrystn. in the presence of 0.5 cc. AcOH gave colorless crystals, m. 126-7°; the free base dissolved with heating in concentrated HCl on the steam bath, decolorized, and cooled deposited the HCl salt, colorless transparent plates, m. 168-73°; turned lemon-yellow after several days.

L38 ANSWER 33 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1956:12242 HCAPLUS

DOCUMENT NUMBER: 50:12242

ORIGINAL REFERENCE NO.: 50:2534d-i,2535a-i,2536a-b

TITLE: The preparation of substituted hydrazines. I. Alkylhydrazines via alkylsydnones

AUTHOR(S): Fugger, Joseph; Tien, Jack M.; Hunsberger, I. Moyer

CORPORATE SOURCE: Antioch Coll., Yellow Springs, O.

SOURCE: Journal of the American Chemical Society (1955), 77, 1843-8

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

OTHER SOURCE(S): CASREACT 50:12242

IT 3182-82-9, Glycine, N-butyl-, hydrochloride 56676-69-8, Glycine, N-hexyl-, hydrochloride (preparation of)

RN 3182-82-9 HCAPLUS

CN Glycine, N-butyl-, hydrochloride (7CI, 8CI, 9CI) (CA INDEX NAME)

n-BuNH-CH<sub>2</sub>-CO<sub>2</sub>H

● HCl

RN 56676-69-8 HCAPLUS

CN Glycine, N-hexyl-, hydrochloride (9CI) (CA INDEX NAME)

Me-(CH<sub>2</sub>)<sub>5</sub>-NH-CH<sub>2</sub>-CO<sub>2</sub>H

● HCl

AB The conversion of an alkylamine to an alkylhydrazine via the corresponding N-alkylglycine, N-nitroso-N-alkylglycine, and N-alkylsydnone is shown to constitute an acceptable preparative method in the cases of PhCH<sub>2</sub>NHNH<sub>2</sub>

(I), BuNHNH<sub>2</sub> (II), and C<sub>6</sub>H<sub>13</sub>NHNH<sub>2</sub> (III). The infrared spectra of N-benzylsydnone (IV), N-butylsydnone (V), and N-hexylsydnone (VI) are presented. ClCH<sub>2</sub>CO<sub>2</sub>Et (122 g.) and 214 g. PhCH<sub>2</sub>NH<sub>2</sub> in 1 l. C<sub>6</sub>H<sub>6</sub> refluxed 5 hrs. with stirring, the mixture filtered, the filtrate distilled to leave 154 g. PhCH<sub>2</sub>NHCH<sub>2</sub>CO<sub>2</sub>Et, yellow oil, the residue filtered, the crude ester added dropwise with stirring during 15 min. to 63.6 g. NaOH in 300 cc. H<sub>2</sub>O, the yellow solution refluxed 45 min. washed with Et<sub>2</sub>O, and acidified with concentrated HCl to pH 2, the resulting white suspension of PhCH<sub>2</sub>NHCH<sub>2</sub>CO<sub>2</sub>H treated at 0° with stirring during 0.5 hr. with 55.2 g. NaNO<sub>2</sub> in 100 cc. cold H<sub>2</sub>O, the mixture stirred 2 hrs., brought to pH 2 with concentrated HCl, refrigerated 1 hr., and filtered, and the filter residue dried in vacuo over KOH yielded 139 g. crude PhCH<sub>2</sub>N(NO)CH<sub>2</sub>CO<sub>2</sub>H (VII). The VII heated 5 hrs. with stirring on the steam bath with 685 cc. Ac<sub>2</sub>O, the resulting dark red solution filtered, and the filtrate evaporated in vacuo yielded 115 g. crude IV, red-brown oil, which solidified in an ice bath on scratching. The crude IV heated 4.5 hrs. on a steam bath with 1 l. 1:1 HCl, the red solution filtered, the clear filtrate concentrated to less than

100

cc. and filtered, and the residual crude I.HCl (56.8 g.) recrystd. twice from boiling EtOH yielded 14.6 g. pure I.HCl, m. 108-10.5°; and from mother liquor an addnl. 6.1 g. I.HCl. BrCH<sub>2</sub>CO<sub>2</sub>Et (68 cc.) in 100 cc. C<sub>6</sub>H<sub>6</sub> added portionwise with swirling and cooling to 120 cc. BuNH<sub>2</sub> in 300 cc., the mixture refluxed 2 hrs. on a steam bath, cooled, and filtered, the residual HBr salt (59 g.) washed with 80 cc. C<sub>6</sub>H<sub>6</sub>, the combined filtrate and washing concentrated in vacuo until white fumes appeared, the residue refluxed 25 min. with 28 g. NaOH in 120 cc. H<sub>2</sub>O, the cooled alkaline solution extracted with Et<sub>2</sub>O, the aqueous layer acidified with cooling to pH 2 with concentrated

HCl, and the mixture refrigerated and concentrated consecutively yielded 68.9 g.

crude BuNHCH<sub>2</sub>CO<sub>2</sub>H.HCl (VIII).HCl, snow-white needles and plates. Crude VIII.HCl (1 g.) in 10 cc. concentrated HCl warmed slightly on the steam bath

and

filtered, the filtrate refrigerated, and this process repeated 3 times gave pure VIII.HCl, m. 204-5°. C<sub>6</sub>H<sub>13</sub>NH<sub>2</sub> and BrCH<sub>2</sub>CO<sub>2</sub>Et gave in exactly the same manner crude C<sub>6</sub>H<sub>13</sub>NHCH<sub>2</sub>CO<sub>2</sub>H.HCl (IX.HCl); the alkaline

solution

of the IX.HCl swirled with cooling with 90 cc. concentrated HCl and 100 g. chopped ice precipitated immediately 81.0 g. IX.HCl, tiny yellowish white flakes;

refrigeration of the mother liquor gave an addnl. 4.8 g. IX.HCl. Crude IX.HCl (1 g.) in 10 cc. H<sub>2</sub>O treated with 1 cc. concentrated HCl, and the resulting precipitate treated 3 times in the same manner gave pure IX.HCl, snow-white flakes, m. 210-17°. Crude IX.HCl (1 g.) recrystd. from 20 cc. 1:1 MeOH-Me<sub>2</sub>CO or 40 cc. glacial AcOH gave the pure salt. VIII.HCl (78.0 g.) in 300 cc. H<sub>2</sub>O treated during 0.5 hr. at -4 to -5° with 37.5 g. NaNO<sub>2</sub> in 100 cc. H<sub>2</sub>O, the mixture stirred 2 hrs., the oily bottom layer drawn off and dissolved in Et<sub>2</sub>O, and the solution filtered, dried, and evaporated gave 62.0 g. crude BuN(NO)CH<sub>2</sub>CO<sub>2</sub>H (X), yellow granular powder. Crude X (8.0 g.) crystallized from a small amount Et<sub>2</sub>O gave 4.53 g. nearly

white

granular solid, m. 60-2°, which recrystd. from aqueous EtOH or Et<sub>2</sub>O-petr. ether gave pure X, long snow-white flakes, m. 61-2°. An alkaline solution of IX prepared from 0.60 mole BrCH<sub>2</sub>CO<sub>2</sub>Et, cooled, treated

with

stirring with 49.7 g. NaNO<sub>2</sub> in 100 cc. H<sub>2</sub>O in 1 portion followed dropwise during 1.25 hrs. by 90 cc. concentrated HCl diluted with 50 g. ice, stirred 1

hr.,

and adjusted with concentrated HCl to pH 2.0, the resulting brown oily top layer

of crude  $C_6H_{13}N(NO)CH_2CO_2H$  (XI), (74.8 g.) allowed to stand, and the solidified yellow granular powder recrystd. from Et<sub>2</sub>O and then aqueous EtOH or petr. ether-Et<sub>2</sub>O gave pure XI, long white flakes, m. 79-80°. Crude X (40 g.) in 236 cc. Ac<sub>2</sub>O heated 3 hrs. on the steam bath, the mixture kept 1 day at room temperature, and the excess Ac<sub>2</sub>O distilled off gave 33 g. crude V; an 8-g. sample distilled yielded 4.5 g. pure V, pale yellow oil, b<sub>2</sub> 165-7°. X (0.362 mole) heated 3 hrs. with only 1.09 moles Ac<sub>2</sub>O gave nearly identical results. Crude yellow-white XI prepared from 0.20 mole BrCH<sub>2</sub>CO<sub>2</sub>Et dissolved in Et<sub>2</sub>O, the extract dried over Na<sub>2</sub>SO<sub>4</sub>, treated with 190 cc. Ac<sub>2</sub>O, kept 1 day at room temperature, and evaporated on the steam bath, the residual oil refluxed 3 hrs., the excess Ac<sub>2</sub>O removed in vacuo, and the clear brown oil dried in vacuo over KOH and P<sub>2</sub>O<sub>5</sub> yielded 23 g. crude VI, which on distillation yielded 18 g. pure VI, b<sub>0.43</sub> 170-6° (redistd., b<sub>0.09</sub> 141-3°). XI (0.334 mole) dissolved in 1.14 moles warm AcOH, and the brown solution heated 2 hrs. on the steam bath after standing overnight yielded 93% VI. Crude V (40.5 g.) mixed with 80 cc. concentrated HCl, the mixture heated 2 hrs. on the steam bath, cooled to room temperature, treated with 20 cc. concentrated HCl, refrigerated overnight, treated with dry HCl to beginning crystallization, refrigerated again, and filtered, the residue washed with 1:1 MeOH-Et<sub>2</sub>O to yield 22 g. nearly white transparent needles, the filtrate decolorized with Norit A, saturated below 0° with dry HCl, refrigerated several days, neutralized with solid Na<sub>2</sub>CO<sub>3</sub>, and extracted with Et<sub>2</sub>O, a part of the extract treated with dry HCl, and the white precipitate filtered off gave II.HCl; the remainder of the extract treated in EtOH with (CO<sub>2</sub>H)<sub>2</sub> yielded the oxalate of II. Distilled V (4.4 g.) heated 2.5 hrs. with concentrated HCl, the yellow solution treated after 2 hrs. with an addnl. 10 cc. HCl, and the solution cooled and saturated with dry HCl yielded 3.1 g. II.HCl, thin white plates, m. 149-54°. II.HCl (3.0 g.) treated with 15 cc. 25% aqueous Na<sub>2</sub>CO<sub>3</sub>, the alkaline mixture extracted with Et<sub>2</sub>O, and the extract distilled gave 1.0 g. V, colorless liquid with an amine odor, b<sub>20</sub> 82-5°. Crude VI.HCl (40.7 g.) and 80 cc. concentrated HCl heated 2 hrs. on the steam bath, the mixture treated with an addnl. 30 cc. HCl and refrigerated, the dark brown cake dissolved in about 150 cc. H<sub>2</sub>O, and the solution heated a few min. on the steam bath with about 5 g. Norit, filtered hot, and cooled deposited 19.8 g. III.HCl, fine transparent needles; the mother liquor treated with (CO<sub>2</sub>H)<sub>2</sub> in EtOH gave 18.0 g. III oxalate. The alkaline solution of the Na salt of IX from 0.60 mole BrCH<sub>2</sub>CO<sub>2</sub>Et treated below 0° with 37.2 g. NaNO<sub>2</sub> in 120 cc. H<sub>2</sub>O in 1 portion, the mixture allowed to stand 0.5 hr., treated with 100 cc. concentrated HCl containing 50 g. crushed ice, stirred 1 hr., and extracted with Et<sub>2</sub>O, and the Et<sub>2</sub>O evaporated gave a residue of 88.7 g. XI. XI (83.7 g.) heated 2 hrs. on the steam bath with 126 cc. Ac<sub>2</sub>O, the excess Ac<sub>2</sub>O removed gave 81.5 g. crude VI. Crude VI (64 g.) heated 2 hrs. on a steam bath with 110 cc. concentrated HCl, cooled, neutralized with 25% aqueous NaOH, saturated with K<sub>2</sub>CO<sub>3</sub>, and extracted 8 times with Et<sub>2</sub>O, the extract dried with K<sub>2</sub>CO, and added to 76 g. (CO<sub>2</sub>H)<sub>2</sub> in 400 cc. 95% EtOH, the mixture allowed to stand overnight, and the yellowish solid filtered off and dried yielded 55.5 g. crude III.(CO<sub>2</sub>H)<sub>2</sub>. Crude III.(CO<sub>2</sub>H)<sub>2</sub> (1.0 g.) recrystd. from 25 cc. hot 9:1 MeOH-EtOH yielded 410 mg. fluffy flakes, m. 171-2°; a 94-mg. sample in 5 cc. hot MeOH evaporated slowly at room temperature yielded 64 mg. large white



needles, m. 173-3.5°; this material dissolved in 5 cc. hot 4; 1 MeOH-EtOH, the solution filtered, and the filtrate poured into a sintered glass funnel gave 26 mg. pure III.(CO<sub>2</sub>H)<sub>2</sub>, transparent needles, m. 174.5-5.5°. II.HCl dissolved in 150-200 cc. H<sub>2</sub>O, neutralized with 30% aqueous NaOH in portions, saturated with solid K<sub>2</sub>CO<sub>3</sub>, and extracted with Et<sub>2</sub>O, the extract dried over K<sub>2</sub>CO<sub>3</sub> and added to 54 g. (CO<sub>2</sub>H)<sub>2</sub> in 320 cc. 95% EtOH, the mixture allowed to stand overnight and filtered to give 18.5 g. crude salt, the mother liquor of the original II.HCl treated in the same manner to give an addnl. 6.3 g. oxalate, and the solid material combined gave 24.8 g. crude II.(CO<sub>2</sub>H)<sub>2</sub>. Crude II.(CO<sub>2</sub>H)<sub>2</sub> (1 g.) recrystd. from 60 cc. hot 9:1 MeOH-EtOH yielded 420 mg. pure material, fine snow white needles; a sample (180 mg.) recrystd. from 20 cc. of the same solvent yielded 144 mg. pure material, white needles, m. 164-5°.

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